



A LiDAR-Based Clustering Method for Automated Atmospheric Boundary Layer Height Detection Over Complex Terrain

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Abstract. The planetary boundary layer height (PBLH) is a critical physical parameter for characterizing atmospheric dynamics, thermodynamic structures, and pollutant dispersion. LiDAR, as a high-spatiotemporal-resolution remote sensing tool, is widely employed to retrieve PBLH by analyzing backscatter signals that reflect aerosol concentrations. However, in complex terrains such as valleys, the boundary layer structure exhibits significant non-homogeneity and complexity due to local terrain-induced dynamic effects. This complexity renders traditional retrieval methods susceptible to interference from multi-layer aerosols and low signal-to-noise ratios (SNR). To address these challenges, this paper proposes an automated identification method—the Physics-Constrained Adaptive K-means (PCA-Kmeans) clustering analysis—specifically tailored for complex valley environments. The PCA-Kmeans framework first constructs a multi-feature scoring mechanism—incorporating signal intensity, vertical gradients, temporal continuity, and vertical compactness—to apply physical constraints for screening clustering results. Subsequently, a gradient-weighted selection and median smoothing strategy are introduced to pinpoint the PBLH from the optimal cluster, effectively mitigating the interference of complex stratification induced by valley topography. The proposed method was validated using LiDAR observation data from the Vipava Valley, Slovenia, from 2018 to 2019. Using Radiosonde (RS) measurements as the reference benchmark, a comparative analysis was conducted between the PCA-Kmeans method, the Gradient Method (GRD), and the Standard Deviation Method (STD). The results indicate that in valley atmospheres influenced by thermally driven local circulations, the PCA-Kmeans method demonstrates superior robustness under low SNR and multi-layer aerosol conditions. The inversion results show higher consistency with RS data, effectively overcoming the identification biases of traditional algorithms caused by residual aerosol layers. This study provides a reliable and automated technical solution for the long-term monitoring of valley boundary layers under the influence of complex local circulations.

1 Introduction

The planetary boundary layer (PBL) is the lowest part of the atmosphere significantly influenced by surface friction, with its height (PBLH) typically fluctuating between hundreds of meters and several kilometers (Su et al., 2017). Within the PBL, momentum, heat, moisture, and pollutants are continuously exchanged with the Earth's surface through intense turbulence, exhibiting strong diurnal variation and spatial heterogeneity (Zhang et al., 2020). The planetary boundary layer height (PBLH) is a critical parameter determining atmospheric environmental capacity and pollutant dispersion capability. It not only directly controls the accumulation and dilution of near-surface pollutants but also regulates local weather changes and long-term climatic effects by influencing moisture transport and aerosol distribution. Studies have shown that under the same emission intensity, variations in PBLH can result in multi-fold differences in ground-level pollutant concentrations (Li et al., 2021). Furthermore, PBLH is closely related to variables such as vertical compactness and the ventilation coefficient (the product of mixing layer height and wind speed, reflecting pollutant dispersion capacity), which is of great significance for air quality



40 modeling, pollution early warning, and climate model parameterization (Garratt, 1994; Tian et al., 2026). Simultaneously, by regulating the upward transport of moisture and aerosols into the free atmosphere, PBLH indirectly affects cloud formation height, optical thickness, and precipitation potential (Guo et al., 2016). Accurate acquisition of PBLH can not only significantly enhance numerical weather prediction but also provide reliable support for practical applications such as wind energy development and aviation safety (Seidel et al., 2010; Gultepe et al., 2015).

45 Under complex terrain conditions, the structure and evolution of the PBL exhibit a high degree of complexity. Driven by the combined effects of terrain-induced thermal circulations and dynamic lifting, unique local circulation systems often form in valleys and basins. Finnigan et al. (2020) pointed out that slope flows, separated flows, and gravity wave perturbations cause turbulent mixing within the boundary layer to deviate significantly from local equilibrium, making it difficult for a single physical criterion to accurately define its height (Finnigan et al., 2020). Lehner and Rotach (2018) emphasized that terrain-
50 induced circulation interference undermines the horizontal homogeneity assumption relied upon by traditional inversion algorithms, often resulting in multi-layered atmospheric structures (Lehner & Rotach, 2018). Under such intricate stratification features, the coupling of local circulations with background wind fields increases the difficulty of identifying the boundary layer top. Furthermore, the characteristic cold air pools and valley-bottom inversions in mountainous regions lead to more persistent near-surface stable stratification, further exacerbating the challenges of PBLH retrieval. Typically, PBLH can be
55 obtained using various tools and methods, such as radiosonde (RS), microwave radiometers (MWR), wind profiler radars (WPR), and LiDAR (Caicedo et al., 2020). Although RS observations are regarded as the reference benchmark, their low temporal sampling rate makes it difficult to capture the rapid evolution of the boundary layer (Seidel et al., 2010). In contrast, LiDAR has become the most widely used ground-based remote sensing means for capturing the dynamic features of PBLH in complex terrain due to its superior spatiotemporal resolution (Dang et al., 2019).

60 Traditional LiDAR-based retrieval methods for PBLH primarily rely on signal discontinuities caused by the sharp decrease in aerosol concentration near the top of the boundary layer. Representative approaches include the Gradient Method (Emeis et al., 2008), Variance Method (Hooper and Eloranta, 1986), Wavelet Covariance Transform (WCT) (Gamage and Hagelberg, 1993), and Ideal Profile Fitting (Steyn et al., 1999). Steyn et al. (1999) proposed determining the PBLH by minimizing the root-mean-square error (RMSE) between the observed profile and an idealized exponential profile (Steyn et al., 1999). Brooks (2003) adopted the WCT method using the Haar wavelet, automatically locating the PBLH at the maximum
65 covariance between the sliding Haar wavelet and the LiDAR signal (Brooks, 2003). Sawyer and Li (2013) fused the Gradient Method with the Threshold Method for Micro-Pulse LiDAR (MPL) data, improving reliability under complex atmospheric conditions through multi-source validation, including RS data (Sawyer & Li, 2013). However, the stability and generalization capability of these methods decrease significantly when applied to atmospheres with complex terrain or multi-layered
70 structures.

In recent years, researchers have proposed numerous improvements to address the limitations of traditional methods, such as sensitivity to noise, susceptibility to residual layer interference, and the need for manual parameter tuning. For instance, the DTDS algorithm developed by Roldán-Henao et al. (2024) effectively overcomes the susceptibility of traditional WCT to residual layers by distinguishing thermodynamic stability and introducing dynamic criteria, significantly enhancing retrieval
75 accuracy and vertical structural consistency for CATS spaceborne LiDAR (Roldán-Henao et al., 2024). Macatangay et al. (2025) integrated a temperature-constrained dynamic maximum analysis height into the Haar WCT framework, effectively avoiding the misidentification of residual layer tops as PBLH during nighttime transition periods (Macatangay et al., 2025). Christopoulos et al. (2025) noted that, compared to traditional WCT methods, optimized machine learning models significantly reduce estimation errors and exhibit stronger environmental adaptability when processing airborne LiDAR data (Christopoulos et al., 2025). However, under complex terrain conditions (e.g., valleys and basins), single optical signals remain highly
80 vulnerable to interference from terrain-induced multi-layer aerosol structures, high aerosol optical depth (AOD), local cloud contamination, and the complex coupling between residual layers and the true boundary layer. Furthermore, the increased



parameter sensitivity under these conditions hinders fully automated and robust retrieval, limiting the applicability of traditional methods in diverse geographical environments. Leveraging their advantages in processing non-linear signals, machine learning methods have increasingly become vital for aerosol LiDAR data inversion. Early studies, such as Toledo et al. (2014), pioneered the application of clustering analysis to LiDAR signals, validating the efficacy of K-means in identifying aerosol stratification features through standardized preprocessing (Toledo et al., 2014). Building on this, Rieutord et al. (2021) proposed the unsupervised clustering algorithm KABL; by comparing it with the supervised method ADABL, they demonstrated that unsupervised approaches offer superior self-adaptability and cross-site generalization in the absence of prior labels (Rieutord et al., 2021). Subsequently, Liu et al. (2022) proposed the Mahalanobis-based K-nearest-means (MKnm) algorithm, achieving reliable PBLH estimation for cloudy or residual-layer conditions using single-band aerosol LiDAR data (Liu et al., 2022). To overcome the information limitations of single-instrument detection, researchers have recently focused on the deep integration of multi-source observations with supervised learning frameworks. For example, Li et al. (2023) combined Random Forest with traditional gradient methods, introducing multi-dimensional meteorological variables to significantly enhance PBLH retrieval accuracy under complex aerosol backgrounds (Li et al., 2023). Zhang et al. (2025) further utilized the LightGBM model, fusing multi-source data—including micro-pulse LiDAR, Doppler LiDAR, and thermodynamic profiles—to significantly improve PBLH estimation precision across various vertical compactness conditions (Zhang et al., 2025). However, the aforementioned methods are predominantly validated under flat terrain or urban site conditions. In complex terrains such as valleys, their performance is still significantly hindered by local circulations, shallow stable layers, and multi-layer aerosol structures. Although supervised learning models based on multi-source data demonstrate high precision, they rely heavily on high-quality labeled data, and their transferability across different geographical environments remains limited. In contrast, unsupervised clustering algorithms, represented by K-means, offer unique advantages in terms of computational efficiency, zero-label dependency, and performance in resource-constrained scenarios. These methods are not only suitable for real-time monitoring but can also serve as initial estimates or preprocessing modules for more complex models. Therefore, enhancing the robustness of unsupervised algorithms in complex terrain by introducing physical constraints and multi-dimensional features—while retaining their inherent self-adaptability—represents a critical direction for advancing the universality of PBLH retrieval technology.

Based on the aforementioned context, this study aims to overcome the typical challenges encountered in LiDAR-based PBLH retrieval under the complex terrain conditions of valley regions. These challenges include stratification aliasing caused by multi-layer aerosol structures, the difficulty of distinguishing between residual layers and the true boundary layer top, indistinct features under weak-signal conditions, and cloud interference. Accordingly, we propose an improved retrieval method—the Physics-Constrained Adaptive K-means (PCA-Kmeans). Building upon the traditional unsupervised clustering framework, the PCA-Kmeans method introduces a multi-feature fusion strategy that integrates backscatter signals and their gradient information to enhance the identification capability of boundary layer structures. Simultaneously, robust identification of the target layer is achieved through adaptive cluster number selection and a cluster evaluation criterion based on physical characteristics. Furthermore, the method incorporates temporal continuity constraints to suppress non-physical mutations in the retrieval results and employs multi-time-scale processing to enhance stability and consistency. While maintaining the inherent advantage of unsupervised methods in terms of zero-label dependency, the proposed approach effectively improves the robustness and applicability of PBLH retrieval in complex terrain.

2 Source and description of experimental data

2.1 Topographic features of Vipava

The Vipava Valley, located in southwestern Slovenia, is a semi-enclosed basin situated approximately 25 km from the Adriatic coast. It is bounded to the south by the Karst Plateau (with elevations up to 300 m above sea level) and to the north



by the steep ridges of the Trnovo Plateau (reaching altitudes up to 1000 m). Surrounded by mountains on three sides, the valley facilitates the accumulation of aerosols and the evolution of complex boundary layer structures. The region exhibits complex aerosol dynamics driven by factors such as valley topography, anthropogenic pollution (primarily from residential heating systems and traffic emissions), and natural aerosols (including mineral dust and sea salt). Consequently, this site is particularly well-suited for investigating PBLH variations under complex terrain conditions (Wang et al., 2022).



Figure 1: Study area terrain location. Research sites are marked with red landmarks. (Map data: © 2026 Google, available at <https://www.google.com/maps/>)

2.2 Lidar system

The LiDAR observation data employed in this study were obtained from a dual-wavelength polarization-Raman LiDAR system deployed in the Vipava Valley, Slovenia (45.87°N, 13.90°E; 125 m above sea level) (Wang et al., 2019). Operating at 355 nm and 1064 nm, the system is characterized by its capability for remote operation and a high, all-weather duty cycle. The LiDAR system provides vertical profiles of atmospheric backscatter with a vertical resolution of approximately 18 m, a temporal resolution of 1 s and a maximum detection range of up to 20 km. For this research, raw range-squared corrected signal (RSCS) data from the 1064 nm elastic backscatter channel were utilized.

2.3 RS

To evaluate the accuracy of the LiDAR-based PBLH estimations, a comparative analysis was performed against RS data. The RS data were obtained from the Rivolto station (113 m above sea level), located approximately 67 km from the Ajdovščina LiDAR site. Due to the significant differences in topographical conditions between the two locations, the RS results were utilized as a reference benchmark rather than an absolute ground truth. The altitudes of both the LiDAR and RS profiles were corrected relative to the ground level at the Ajdovščina site. RS are typically launched twice daily at 00:00 and 12:00 UTC. The local time zone follows UTC+2 during Central European Summer Time (CEST) and UTC+1 during Central European Time (CET). To synchronize the PBLH estimations from the two sources, the LiDAR data were averaged over a 10-minute window centered at the RS launch time (i.e., ±5 minutes) for the comparative analysis (Wang et al., 2022).

3 Method

This study employs multiple methods to estimate the PBLH, including the Gradient Method (GRD), the Standard Deviation Method (STD), and the proposed multi-feature method based on K-means clustering, with validation performed against RS results. The Range Corrected Signal (RCS) is obtained after subtracting background noise (Wandinger, 2005). Cloud contamination is mitigated using an adaptive logarithmic threshold combined with vertical gradient criteria, while the PBL search range is constrained within a typical boundary layer height interval.



To further enhance the stability of the retrieval results, a unified temporal continuity constraint and a post-processing smoothing strategy are incorporated into all algorithms. This constraint mechanism ensures that the identified results conform to the physical laws of atmospheric evolution by limiting the magnitude of PBLH variations between adjacent time steps. If the difference between the current estimated height and the previous valid one exceeds a reasonable mutation threshold based on atmospheric dynamics, a bounded constraint is applied to the height increment; this limits the jump magnitude while preserving the original evolutionary trend. If the variation falls within a reasonable range, an exponential weighted moving average is employed for smooth updates, thereby reducing the influence of instantaneous noise and cloud-edge interference. This ensures objectivity and scientific rigor in the evaluation across different retrieval methods. Subsequently, the differences in estimation results and their underlying causes under various meteorological conditions are analyzed. Finally, an operational procedure for LiDAR-based PBLH retrieval tailored for valley terrain is proposed.

3.1 Traditional methods

3.1.1 Gradient method

The aerosol concentration within the planetary boundary layer is significantly higher than that in the free atmosphere, resulting in a distinct attenuation of the LiDAR backscatter signal at the top of the boundary layer. The Gradient Method (GRD) determines the PBLH by identifying the maximum negative gradient of the vertical RCS profile (Emeis et al., 2008).

$$\text{PBLH}_{\text{GRD}} = \operatorname{argmax}_z \left[-\frac{d(\text{RCS}(z))}{dz} \right] \quad (1)$$

where PBLH_{GRD} denotes the boundary layer height estimated by the GRD method, and $\text{RCS}(z)$ represents the LiDAR signal at altitude z after background subtraction and range correction.

3.1.2 Standard deviation method

In the entrainment zone, turbulent mixing leads to intense fluctuations in aerosol concentration. The Standard Deviation Method (STD) determines the PBLH by calculating the temporal standard deviation of the RCS across multiple profiles at each altitude over a specific time interval, identifying the height corresponding to the maximum STD value (Hooper & Eloranta, 1986).

$$\text{STD}(z) = \sqrt{\frac{1}{N} \sum_{i=1}^N [\text{RCS}(z, t_i) - \overline{\text{RCS}}(z)]^2} \quad (2)$$

where $\text{RCS}(z, t_i)$ denotes the LiDAR backscatter signal at altitude z and time t_i , and $\overline{\text{RCS}}(z)$ represents the average value of N consecutive profiles for each 30 min time interval. The altitude z corresponding to the maximum standard deviation is identified as the center of the entrainment zone, which defines the top of the atmospheric boundary layer.

3.1.3 K-means

K-means is a classical unsupervised learning algorithm that partitions data into clusters based on feature similarity. In this study, altitude and normalized range-corrected signal (RCS) are used as clustering features. After Z-score standardization, the candidate cluster numbers range from 3 to 5, and the optimal number is determined using the silhouette coefficient. The clustering objective is to minimize the within-cluster sum of squared distances:

$$J = \sum_{j=1}^K \sum_{x_i \in C_j} \|x_i - \mu_j\|^2 \quad (3)$$

where K is the number of clusters, C_j represents the j -th cluster, x_i denotes a feature vector, and μ_j is the corresponding cluster center.



After clustering, the most frequent cluster label at each altitude is used to construct a vertical cluster-label profile. The first vertically persistent cluster transition is then identified, and its midpoint is used to estimate the PBLH.

$$\text{PBLH}_{\text{K-means}} = \frac{z_{i-1} + z_i}{2} \quad (4)$$

where z_i and z_{i-1} represent the adjacent altitudes at the identified cluster transition. Finally, temporal averaging and median filtering are applied to reduce short-term fluctuations.

3.1.4 RS

RS observations serve as reference measurements for evaluating LiDAR-derived PBLH estimates. Generally, the position of the maximum positive gradient of the virtual potential temperature (θ_v) derived from RS profiles is defined as the accurate PBLH. While this method is regarded as the reference standard, it is constrained by the sampling frequency (typically twice daily) and spatial representativeness, given that the RS station in this study is located approximately 67 km from the LiDAR site (Zhou et al., 2025).

$$\text{PBLH}_{\text{RS}} = \text{argmax}_z \left(\frac{d(\theta_v(z))}{dz} \right) \quad (5)$$

where $\theta_v(z)$ is the virtual potential temperature at height z above ground level, and argmax_z identifies the height of the maximum positive vertical gradient.

3.2 PCA-Kmeans

Although conventional K-means can identify aerosol stratification through unsupervised clustering, its reliance on statistical similarity alone makes it difficult to distinguish the actual PBL top from other aerosol-layer transitions, particularly under complex valley conditions. To address this limitation, the proposed PCA-Kmeans method incorporates multidimensional LiDAR features and physically constrained cluster evaluation into the conventional clustering framework. The PCA-Kmeans algorithm for obtaining PBLH using lidar observations is described in the flowchart (Fig. 2).

3.2.1 Multidimensional feature construction and asymmetric weighted normalization

To improve clustering accuracy, this approach effectively eliminates dimensional effects and highlights key physical structures. For each temporal profile, a four-dimensional feature vector is extracted, comprising the altitude (z), normalized RCS (norm RCS), first-order gradient (gradient), and second-order gradient (gradient of gradient). Given the significant disparities in dimensions and numerical ranges among these features, the Z-score method is employed to standardize the feature matrix. To guide the clustering algorithm toward physical mutations rather than simple numerical values, an asymmetric weighting mechanism is introduced post-standardization. A baseline weight of 1.0 is assigned to the altitude and intensity dimensions, while significantly enhanced asymmetric weights (3.0 and 1.5) are applied to the first-order and second-order vertical gradients, respectively.

3.2.2 Dynamic clustering for atmospheric stratification

K-means unsupervised clustering is performed on the weighted and standardized feature matrix. Given that the vertical structure of a typical atmosphere generally comprises the mixed layer, the entrainment zone, and the free atmosphere—with increased complexity in the presence of clouds or residual layers—this approach restricts the number of clusters (k) to a range between 3 and 5, of which the fixed value was used in previous study [23]. This range ensures coverage of the primary physical structures while avoiding over-segmentation. Within this candidate range, the silhouette coefficient is employed to evaluate the clustering results. The value that yields the maximum average silhouette coefficient is selected as the optimal number of



clusters. By maximizing intra-class compactness and inter-class separation, an adaptive and optimized partitioning of the atmospheric vertical structure can be achieved.

3.2.3 Physical-constraint-based scoring mechanism and PBLH extraction

To precisely identify the layer corresponding to the top of the boundary layer from the clustering results, a multi-factor physical-constraint scoring function is constructed to perform a comprehensive evaluation of each cluster:

$$Score = (w_1 S_{int} + w_2 S_{grad} + w_3 S_{time} + w_4 S_{stab}) \quad (6)$$

In this context, S_{int} represents signal intensity, reflecting aerosol concentration; S_{grad} denotes the gradient, characterizing the abrupt change at the top of the boundary layer; S_{time} represents continuity, constraining temporal evolution; and S_{stab} describes stability, characterizing the structural compactness of the layers. To comprehensively evaluate the physical features of each cluster, each sub-scoring item is normalized to the range [0, 1] using min-max normalization. During the sensitivity analysis, the weights are normalized such that $\sum_{i=1}^4 w_i = 1$, while the temporal continuity and stability terms are scaled proportionally to maintain their original relative contribution.

To precisely pinpoint the PBLH from the optimal cluster, the top 15% of points characterized by the strongest negative gradients within the cluster are selected. The median altitude of this subset is then designated as the final PBLH. This strategy preserves the physical significance inherent in the traditional Gradient Method (GRD) while enhancing the robustness of the retrieval results through statistical refinement. Also it is not overly sensitive to small variations in the percentile threshold within this range (See attached supplement file). Lower thresholds tend to overemphasize extreme gradients caused by noise, while higher thresholds may incorporate signals from non-boundary layer structures. Therefore, 15% was selected as a representative value within the optimal range, balancing stability and representativeness.

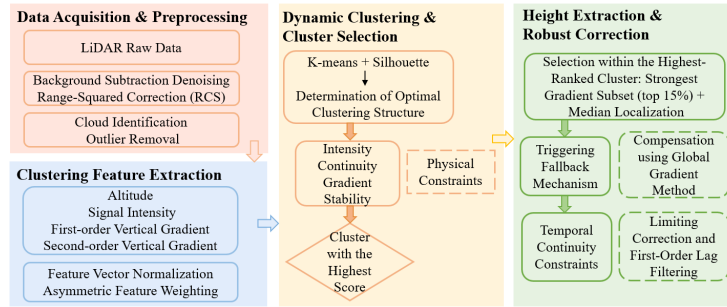


Figure 2: Flowchart of the PCA-Kmeans Algorithm for obtaining PBLH using lidar observations.

3.3 Error evaluation method

The retrieval error is defined as the difference between the estimated PBLH and the RS reference value ($\Delta H = H_{retrieved} - H_{ref}$). To quantify the performance, the following metrics are utilized (Krishnamurthy et al., 2021):

(1) Root mean square error (RMSE)

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (H_{retrieved,i} - H_{ref,i})^2} \quad (7)$$

RMSE characterizes the overall deviation level between the retrieval results and reference values, exhibiting higher sensitivity to large outliers. It serves as a core indicator for assessing the global precision of the method.

(2) Mean bias (Bias)

$$Bias = \frac{1}{n} \sum_{i=1}^n (H_{retrieved,i} - H_{ref,i}) \quad (8)$$



255 Bias measures the systematic error, indicating the tendency of the method to either overestimate (positive Bias) or underestimate (negative Bias) the PBLH. In an ideal scenario, the Bias should approach zero.

(3) Standard Deviation (Std)

$$\text{Std} = \sqrt{\frac{1}{n} \sum_{i=1}^n [(H_{\text{retrieved},i} - H_{\text{ref},i}) - \text{Bias}]^2} \quad (9)$$

260 The Std describes the dispersion of the error, reflecting the stability of the retrieval results. A smaller Std indicates lower error volatility and higher methodological stability.

Furthermore, to analyze the distribution characteristics of the error, a histogram of ΔH is constructed and fitted with a Gaussian function. This analysis determines whether the error is zero-centered and evaluates its distribution pattern, thereby assessing the balance between random errors and structural biases.

265 Regarding consistency assessment, linear regression analysis is employed to compare $H_{\text{retrieved}}$ with H_{ref} , with the correlation coefficient (R) and the regression slope being calculated. The correlation coefficient quantifies the degree of linear correlation between the two, while the regression slope reflects the response capability of the retrieval results to the actual magnitude of variation. Ideally, both R and the slope should approach 1, indicating high consistency between the retrieval results and reference values without significant systematic distortion.

270 Furthermore, to evaluate the applicability of the method under diverse atmospheric conditions, the samples are categorized into three scenarios: cloudy, cloud-free, and all-weather. The aforementioned statistical metrics are calculated separately for each category to systematically analyze the robustness of each method in complex environments (e.g., cloud interference).

In summary, the error assessment framework established in this study provides a comprehensive evaluation of methodological performance across multiple dimensions, including error magnitude (RMSE), systematic bias (Bias), stability (Std), and consistency (R and slope).

4 Results and verification

This study analyzes 102 cases from a total of 93 observation days across 2018 and 2019, presenting the application results of three LiDAR-based PBLH retrieval methods—PCA-Kmeans, GRD, and STD—within a valley boundary layer. These results are further validated through a comparative analysis with RS measurements.

280 In this section, the PCA-Kmeans model is compared with the traditional GRD and STD models for LiDAR-based PBLH estimation. Four representative weather conditions—typical clear-sky, cloudy, aerosol-stratified and weak-signal scenarios—are selected to analyze the diurnal evolution of the convective boundary layer (CBL). Specifically, the correlation between LiDAR-derived PBLH and RS measurements is rigorously evaluated under clear-sky and cloudy conditions.

4.1 Comparative analysis of LiDAR-derived diurnal PBLH evolution

285 (1) Clear-sky

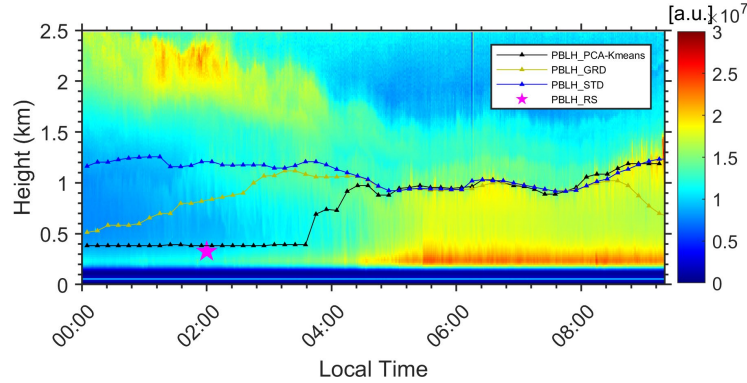


Figure 3: Time-height color plot of LiDAR RCS from 00:00 to 09:15 on April 18, 2018. The PBLH estimated by PCA-Kmeans, GRD, and STD are denoted by black, yellow, and blue lines, respectively. RS measurements are represented by magenta pentagrams.

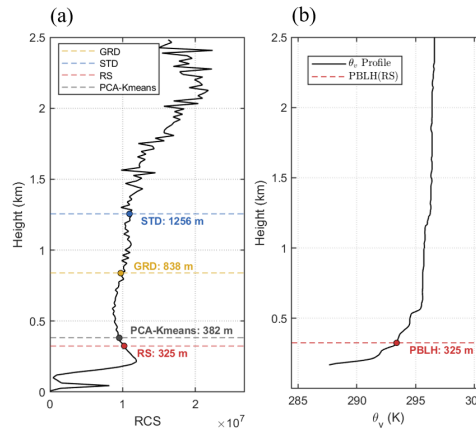


Figure 4: Signal profiles at 02:00 CET on April 18, 2018. (a) 1064 nm RCS profile; (b) Virtual potential temperature profile from RS.

Figure 3 illustrates the transition of the atmospheric boundary layer from a nocturnal stable boundary layer (SBL) to a daytime convective boundary layer (CBL). Prior to 05:00 CET, the atmosphere exhibited a typical nocturnal stable stratification, with a prominent residual layer (RL) located at approximately 1.0 km. Taking 02:00 as an example (Fig. 4), the PBLH observed by RS was 325 m. In contrast, the retrieval results from the traditional GRD and STD methods were 1256 m and 838 m, respectively, representing a significant overestimation of the actual height. This discrepancy stems from the inherent sensitivity of traditional algorithms to signal gradients. Under SBL conditions, due to weak near-surface turbulence, the signal gradient at the top of the residual layer is sharper than that at the actual boundary layer top, causing the algorithms to misidentify the layer interface. In comparison, the PBLH retrieved by the PCA-Kmeans algorithm was approximately 382 m, showing a substantially smaller error relative to the RS observation. These results demonstrate that the multi-dimensional feature space clustering approach can effectively distinguish aerosol layers with different physical properties, thereby differentiating the SBL from the RL in multi-layered structures and achieving more robust PBLH identification.

After sunrise, intensified surface heating triggers a rapid growth phase of the boundary layer after 05:00, which subsequently transitions into a convective boundary layer (CBL). The enhanced convective mixing leads to a more uniform aerosol distribution, while simultaneously forming a distinct concentration jump at the top of the boundary layer. As shown in Fig. 3, the PBLH curves derived from the three methods tend to converge starting from 05:00. This convergence indicates that under convective conditions where signal features at the PBL top are prominent, all three algorithms can accurately identify



the boundary layer height. These findings demonstrate that the PCA-Kmeans method not only overcomes the limitations imposed by complex nocturnal stratification but also maintains high precision during the daytime.

310 (2) Cloudy

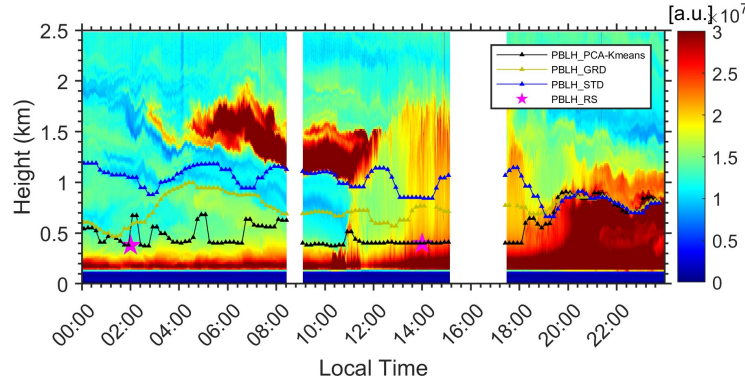


Figure 5: Time-height color plot of LiDAR RCS on August 8, 2018. The line colors are consistent with those in Fig. 3.

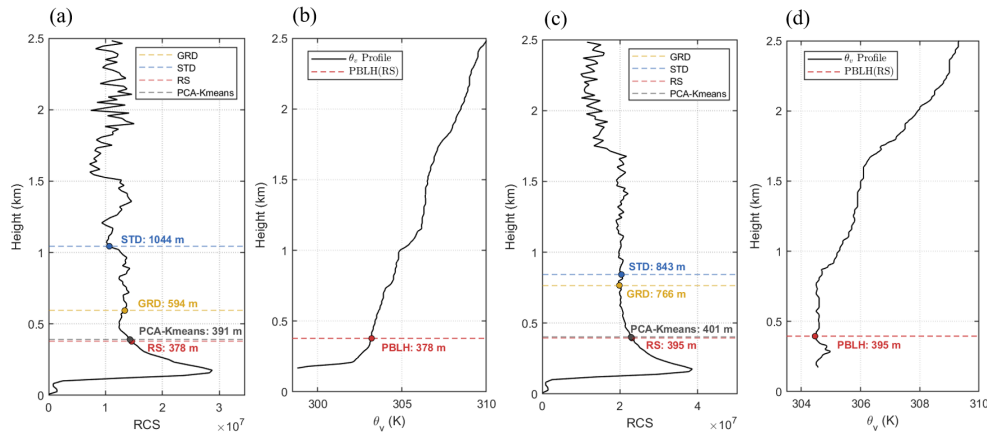


Figure 6: Signal profiles at 02:00 and 14:00 on August 8, 2018. (a) 1064 nm RCS profile at 02:00; (b) Virtual potential temperature profile from RS at 02:00; (c) 1064 nm RCS profile at 14:00; (d) Virtual potential temperature profile from RS at 14:00.

Figure 5 illustrates the diurnal evolution of LiDAR observations on August 8, 2018, which clearly characterizes the PBL features under cloudy summer conditions. Between 05:00 and 12:00, the atmosphere was obscured by dense cloud cover within the 1.0–1.8 km altitude range. Due to the extremely strong backscatter signal gradient generated at the cloud base, the GRD algorithm erroneously identified it as the PBL top. Meanwhile, the STD algorithm was compromised by the signal attenuation zone beneath the clouds, yielding maximum variance at the sharp interface between the strong signal and the attenuation band; consequently, this signal mutation was misidentified as the PBL height. In contrast, the PCA-Kmeans algorithm exhibited remarkable robustness, effectively shielding the interference from these non-physical stratifications through its cloud identification and rejection mechanism. This case study demonstrates the superior stability of the PCA-Kmeans algorithm in complex meteorological scenarios.

As shown in Fig. 6(a), at 02:00 (nocturnal), the PBLH retrieved by GRD and STD were 594 m and 1044 m, respectively, which were clearly interfered with by the elevated residual layer or noise. In contrast, the PCA-Kmeans algorithm yielded a height of 391 m, which is in excellent agreement with the RS-measured height of 378 m shown in Fig. 6(b). At 14:00 (daytime) (Fig. 6c), influenced by clouds and local interference, the GRD and STD results jumped to 766 m and 843 m, representing a severe overestimation. Conversely, the 401 m retrieval result provided by the PCA-Kmeans algorithm remained consistent with the RS-measured height of 395 m shown in Fig. 6(d).



(3) Aerosol stratified

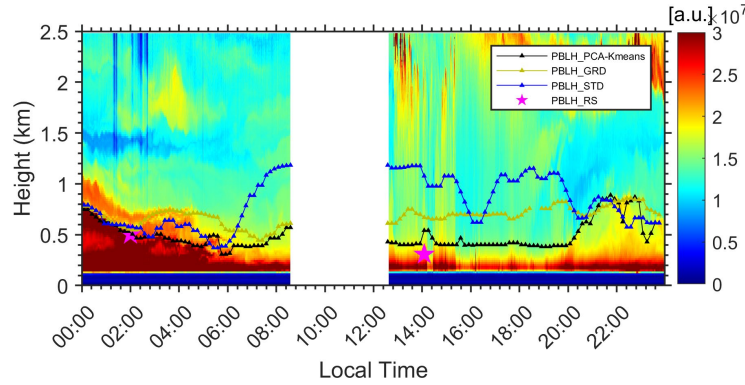


Figure 7: Time-height color plot of LiDAR RCS on August 9, 2018. The line colors are consistent with those in Fig. 3.

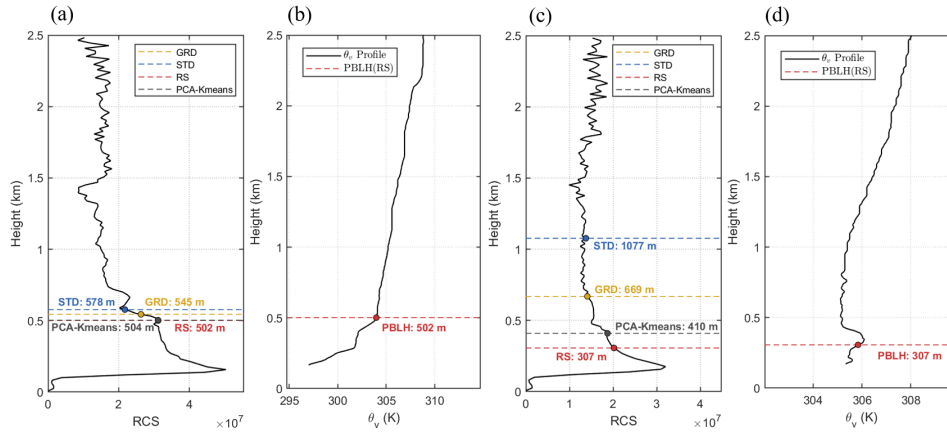


Figure 8: Signal profiles at 02:00 and 14:00 on August 9, 2018. (a) 1064 nm RCS profile at 02:00; (b) Virtual potential temperature profile from RS at 02:00; (c) 1064 nm RCS profile at 14:00; (d) Virtual potential temperature profile from RS at 14:00.

Figure 7 illustrates that the RCS distribution on this day exhibited distinct multi-layer structural characteristics. A shallow stable boundary layer was present beneath an overlying residual layer during the night, while a complex structure featuring a shallow mixed layer superimposed with an elevated aerosol layer was observed during the daytime. Regarding the diurnal characteristics, this case presented an unconventional "night-high, day-low" phenomenon in the retrieval results. This phenomenon may stem from the maintenance of a relatively thick low-level mixed structure by the residual layer at night; conversely, weakened dynamics and restricted development of the thermal mixed layer during the day maintained the PBLH at a lower level. Such multi-layered aerosol distributions significantly increase the identification difficulty for algorithms based on local gradient extrema.

At 02:00 (Fig. 8a), the results from the four methods (GRD: 545 m, STD: 578 m, PCA-Kmeans: 504 m, RS: 502 m) were highly consistent, clustering around 0.500–0.600 km. This reflects the well-defined structure of the stable boundary layer under stagnant weather conditions, characterized by significant near-surface aerosol accumulation. However, the GRD method exhibited fluctuations due to interference from mid-level gradients, while the STD method consistently locked onto the top of the residual layer after 02:00. In contrast, the PCA-Kmeans algorithm consistently focused on the low-level mixed structure, yielding results more consistent with the RS observations. At 14:00 (Fig. 8c), the RS-measured PBLH was 307 m, and the PCA-Kmeans retrieval height was 410 m. Although a certain deviation existed, this result was still markedly superior to those of GRD (669 m) and STD (1077 m). Traditional methods were compromised by strong non-boundary-layer gradient structures during this period, leading to overestimated retrieval heights. This case demonstrates that under complex conditions



characterized by superimposed multi-layer aerosols and significant gradient interference, the PCA-Kmeans method—based
 355 on full-profile feature clustering—can more effectively distinguish the primary mixed layer from the overlying residual layer,
 thereby exhibiting superior robustness and stability.

(4) Weak-signal scenarios

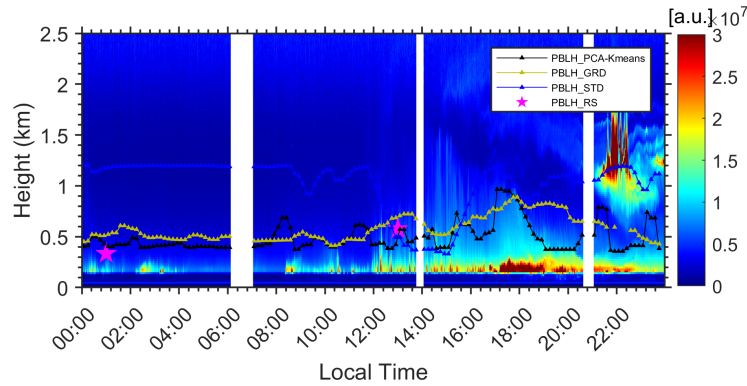


Figure 9: Time-height color plot of LiDAR RCS on January 15, 2019. The line colors are consistent with those in Fig. 3.

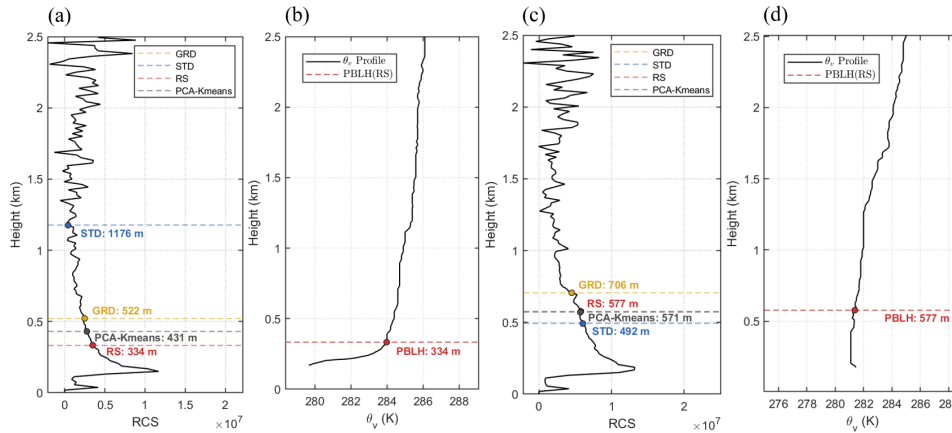


Figure 10: Signal profiles at 01:00 and 13:00 on January 15, 2019. (a) 1064 nm RCS profile at 01:00; (b) Virtual potential temperature profile from RS at 01:00; (c) 1064 nm RCS profile at 13:00; (d) Virtual potential temperature profile from RS at 13:00.

Figure 9 displays the time-height evolution of LiDAR RCS observed during a winter day on January 15, 2019. In winter, atmospheric stratification is typically stable with a lower PBLH, and the vertical diffusion of aerosols is weak; consequently,
 365 the vertical signal contrast is diminished, making identification challenging. In the 01:00 observation (Fig. 10a), the RS-measured PBLH was 334 m, and the PCA-Kmeans retrieval yielded 431 m, which is close to the measured value. In contrast, the results from STD (1176 m) and GRD (522 m) showed significant deviations. During the daytime development phase at 13:00 (Fig. 10c), the RS-observed height was 577 m, while the PCA-Kmeans retrieval was 571 m, showing near-perfect agreement. Conversely, the GRD result (706 m) exhibited a clear overestimation, while the STD result (492 m) showed an
 370 underestimation. This case further demonstrates that under conditions of weak vertical contrast, low signal-to-noise ratio (SNR), and weak gradients typical of winter, the stability and adaptability of PCA-Kmeans are superior to those of traditional gradient-based algorithms.

4.2 Validation of LiDAR-based PBLH retrieval using RS measurements

As summarized in Table I, five approaches were used to analyze the sensitivity of the retrieval method to different
 375 weighting. As the combined weight of intensity and gradient increases from 0.5 to 0.65, the correlation coefficient (R) with



RS results rise from 0.704 to 0.863. However, further increasing this proportion to 0.8 leads to a decrease in performance ($R = 0.827$), indicating that excessive emphasis on primary features amplifies local fluctuations and reduces robustness. These results suggest the existence of an optimal range around 0.65.

In addition, under a fixed total weight of 0.65, adjusting the relative contribution between intensity and gradient shows that assigning a slightly higher weight to the intensity term ($w_1/w_2 \approx 1.17$) achieves the best performance ($R = 0.903$), whereas a lower ratio ($w_1/w_2 \approx 0.86$) results in degraded performance ($R = 0.870$).

Based on these findings, the weights are set following group 4 in Table I, representing a balanced configuration within the optimal and stable parameter regime. The performance remains relatively stable under small perturbations of the weights within this range, indicating that the proposed method is not overly sensitive to parameter selection. But this sensitivity analysis also indicates the optimal weighting coefficients of four physical parameters need to be adjusted under different lidar observation conditions.

Table I

SENSITIVITY ANALYSIS OF WEIGHTING COEFFICIENT CONFIGURATIONS ON RETRIEVAL PERFORMANCE. w_1 (intensity coefficient), w_2 (gradient coefficient), w_3 (temporal continuity coefficient), and w_4 (vertical compactness coefficient)

GROUP	$w_1 + w_2$	$w_3 + w_4$	w_1/w_2	R
1	0.5	0.5	1	0.704
2	0.65	0.35	1	0.863
3	0.8	0.2	1	0.827
4	0.65	0.35	≈ 1.17	0.903
5	0.65	0.35	≈ 0.86	0.870

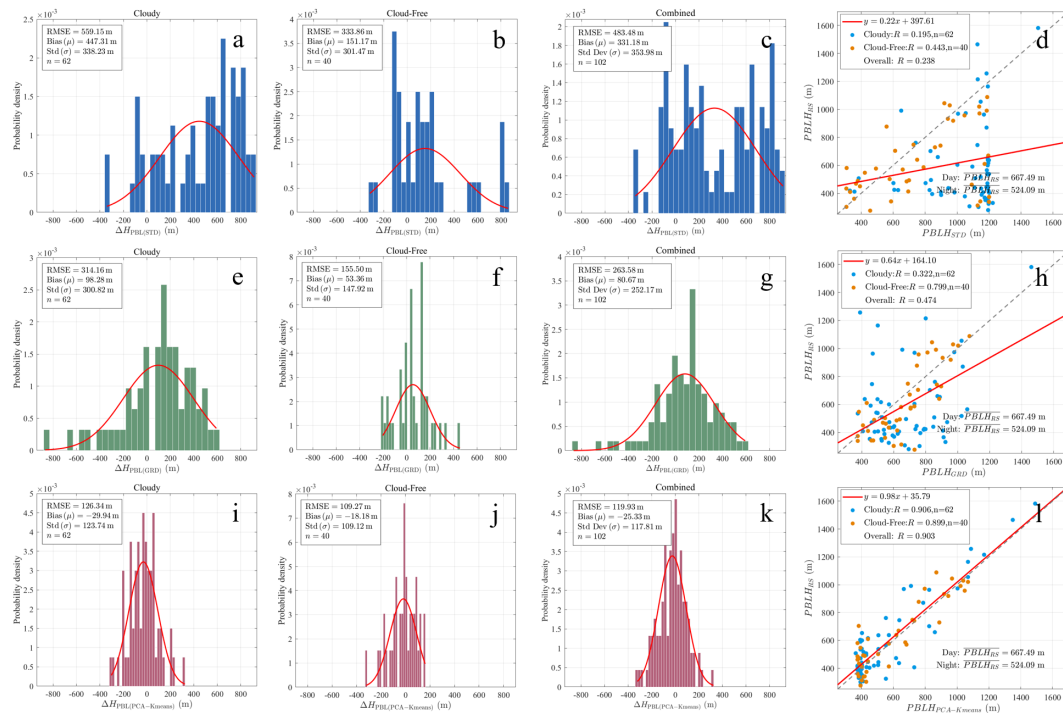


Figure 11: Statistical evaluation and intercomparison of PBLH retrievals from the STD, GRD, and PCA-Kmeans methods against RS observations under different sky conditions. The first to third columns show the probability density functions (PDFs) of the retrieval errors for cloud-free, cloudy, and combined conditions, respectively, while the fourth column presents the corresponding scatter plots with linear regression results. Panels (a–d), (e–h), and (i–l) correspond to the STD, GRD, and PCA-Kmeans methods, respectively.



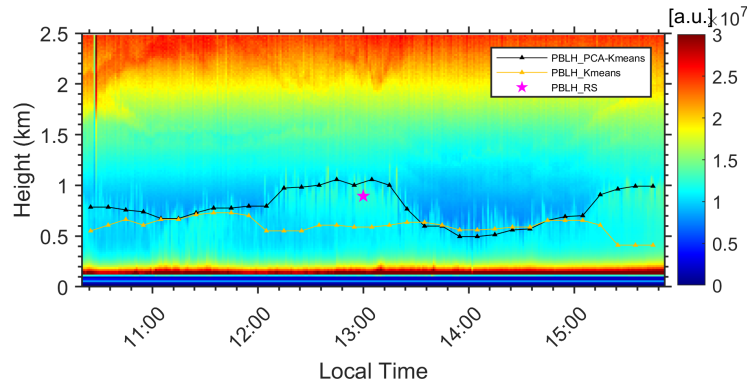
To quantitatively evaluate the precision and robustness of the proposed PCA-Kmeans algorithm, this study conducted a comparative analysis of the retrieval results from the STD and GRD methods, using RS data as the reference. Fig. 11 illustrates the error distribution characteristics and the linear regression relationships between each method and the reference values under various sky conditions. From the error histograms (Cols. 1–3, Fig. 11), it is evident that the error distribution of the PCA-Kmeans method (Figs. 11i–l) is significantly more centralized, with a mean bias of -25.33 m, indicating a minimal systematic bias. Moreover, its distribution profile closely resembles a symmetric Gaussian-like structure, reflecting lower dispersion and more stable error behavior. In contrast, the error distributions of the STD and GRD methods are more widely dispersed, exhibiting pronounced positive biases (331.18 m and 80.67 m, respectively). This suggests a general tendency of traditional methods to overestimate the PBLH, typically stemming from their heavy reliance on abrupt signal gradient or variance mutations. Under conditions of complex aerosol stratification, residual layers, or weak turbulence, these methods are prone to misidentifying non-PBL structures as the boundary layer top. Furthermore, the errors of the PCA-Kmeans method are primarily concentrated within the ± 350 m interval, while traditional methods exhibit a much broader distribution range (up to ± 800 m) (Col. 3, Fig. 11), further demonstrating the significant advantages of the multi-feature clustering strategy in suppressing extreme errors and outlier identification. The scatter plots and linear regression results (Col. 4) further validate these findings. The PCA-Kmeans method achieves a high correlation coefficient ($R = 0.903$ after weighting coefficients optimization), indicating strong consistency with RS observations and maintaining a robust proportional response across different height ranges. Conversely, the correlations for the STD ($R = 0.238$) and GRD ($R = 0.474$) methods are significantly lower, with much more dispersed scatter points, particularly in the high-PBLH range where deviations are more prominent. This indicates that traditional methods have limited capability in characterizing the development of the boundary layer and struggle to stably track its diurnal evolution. The three methods also show marked performance differences under varying meteorological conditions. Under cloudy conditions, the RMSE of the STD method increases significantly to 559.15 m, primarily because strong backscatter signals at the cloud base introduce severe gradient enhancements, leading the algorithm to misidentify the cloud base as the PBL top. While the GRD method partially alleviates this issue, it still suffers from noise amplification and gradient instability. In contrast, the PCA-Kmeans method maintains a low error (RMSE = 126.34 m) under identical conditions, showing negligible change compared to cloud-free conditions (RMSE = 109.27 m), which underscores its reduced sensitivity to cloud interference. The significant reduction in RMSE reflects not only a decrease in the average error level but also the effective suppression of extreme error events, thereby enhancing the overall reliability of the retrieval. Regarding the overall statistical results, the Standard Deviation (Std) of the PCA-Kmeans method on the combined dataset is 117.81 m, compared to 353.98 m and 252.17 m for the STD and GRD methods, respectively. The reduction in Std indicates a more centralized error distribution, implying lower volatility and enhanced continuity in the retrieved time series. This stability is crucial for analyzing the long-term evolutionary characteristics of the planetary boundary layer.

Based on the statistical results, we can also find the PBLHs are significantly influenced by the feature of Vipava Valley, where frequently experiences nocturnal temperature inversions, downslope gust events, and exacerbated pollution from intensive local biomass burning in winter. The PBLH exhibits certain diurnal variations; however, the amplitude remains relatively limited due to the enclosed valley topography, cold air advection that strengthens near-surface stable stratification and suppresses turbulence development, and strong nocturnal inversions (e.g. Fig. 9). Daytime convective mixing typically leads to a slight ascent in the PBLH, with an average of approximately 650 m as shown in Fig. 11, while the boundary layer becomes notably lower under nocturnal stable conditions, generally around 530 m. These characteristics highlight the challenges of accurately measuring the PBLH using LiDAR with traditional methods in such enclosed valley environments, where aerosol stratification, residual layers, and terrain-induced local circulations significantly interfere with the identification and interpretation of the vertical structure.

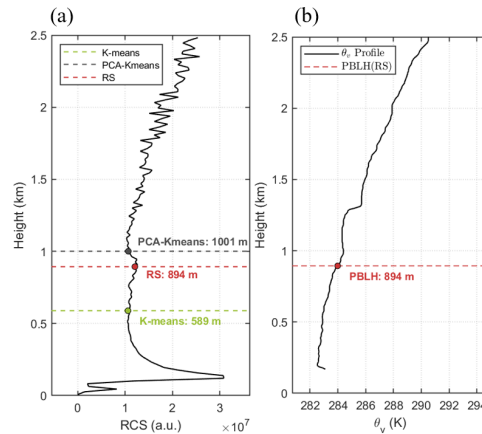


4.3 Ablation analysis of the proposed PCA-Kmeans framework

440 The preceding comparison demonstrates the performance of PCA-Kmeans relative to conventional gradient- and variance-based methods. The following ablation analysis further examines the contribution of the proposed modifications by comparing PCA-Kmeans with conventional K-means. Conventional K-means identifies the PBLH from cluster transitions using altitude and normalized RCS, whereas PCA-Kmeans incorporates additional gradient-based features and a physics-constrained scoring mechanism.



445 **Figure 12: Time-height color plot of LiDAR RCS from 10:20 to 15:50 on January 12, 2018. The PBLH estimated by PCA-Kmeans and K-means are denoted by black and yellow lines, respectively. RS measurements are represented by magenta pentagrams.**



450 **Figure 13: Signal profiles at 13:00 CET on January 12, 2018. (a) 1064 nm RCS profile; (b) Virtual potential temperature profile from RS.**

Figure 12 shows the RCS time–height cross section on January 12, 2018, comparing the PBLH retrieval results of conventional K-means and PCA-Kmeans algorithms. During the active convective period from 12:00 to 13:30, the aerosol mixing layer rose significantly to approximately 1.0 km, a dynamic process successfully captured by the PCA-Kmeans algorithm. In the 13:00 profile (Fig. 13a), PCA-Kmeans retrieved a height of 1001 m, in fair agreement with the RS measurement of 894 m (Fig. 13b). In contrast, conventional K-means was affected by local low-level signal gradients, misidentifying the height as 589 m (Fig. 13a). As convection weakened between 14:00 and 15:00, both algorithms yielded consistent lower-level responses. These results demonstrate that PCA-Kmeans possesses superior capability and robustness for identifying boundary layer tops during intense convective development and rapid aerosol structure changes.

This difference reflects the ambiguity of aerosol-layer transitions in a multilayer atmosphere. A strong internal aerosol transition can produce a distinct cluster boundary even when it does not represent the upper limit of the turbulent boundary layer. Conventional K-means partitions the profile according to statistical similarity and therefore has no explicit criterion for



distinguishing an internal aerosol boundary from the PBL-top transition. PCA-Kmeans introduces vertical-gradient information and evaluates candidate clusters using signal intensity, negative-gradient characteristics, temporal continuity, and vertical compactness. The physical constraints therefore guide the selection among multiple aerosol transitions rather than simply generating a cluster boundary.

The case-level behavior is also supported by the dataset-level statistics. Across all 102 matched samples, conventional K-means achieves an overall correlation coefficient of ($R=0.609$, Fig. 14) with the RS reference, whereas PCA-Kmeans reaches ($R=0.903$, Fig. 111). This improvement indicates that the added physically interpretable features and the physics-constrained selection procedure enhance the consistency of the retrieval with the RS-derived PBLH over the full dataset.

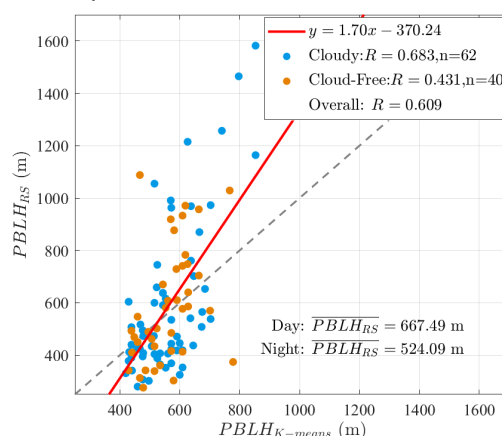


Figure 14: Statistical evaluation and intercomparison of PBLH retrievals from the K-means and PCA-Kmeans methods against RS observations under different sky conditions. The figure presents the corresponding scatter plots and linear regression results.

5 Conclusion

An automated PBLH identification method based on multi-feature K-means clustering integrated with physical constraints and LiDAR signals is proposed for a complex terrain region. The case studies demonstrate that the proposed method exhibits high stability and accuracy under challenging conditions over typical valley topography, such as multi-layer aerosol stratification, and cloud interference. This superiority is particularly pronounced when nighttime stable boundary layers and residual layers are present. Compared with traditional gradient and temporal variance methods, the proposed approach showed smaller discrepancies and stronger correlations with RS observations. Its advantages are primarily reflected in enhanced identification capabilities through multi-feature fusion, improved interpretability via physical constraints, and increased stability through temporal continuity constraints. While GRD and STD offer high computational efficiency, they exhibit sensitivity to noise and complex multi-layer structures. Conversely, the K-means approach enhances robustness through feature integration and constraint mechanisms, albeit at the cost of higher computational complexity. The weighting coefficients of the four LiDAR features affect PBLH retrieval accuracy. Therefore, long-term statistical evaluations at different LiDAR sites may be necessary to improve the generalizability of the proposed method. Such improvements could support more accurate air quality simulations, pollution dispersion forecasting, and a better understanding of boundary layer dynamics in valley environments.

Code and data availability.

Code and data can be provided by the corresponding author on request.



490 **Author contributions.**

Si Liu: Writing – original draft, Formal analysis, Investigation, Methodology, Visualization. Longlong Wang: Writing – review and editing, Supervision, Resources, Project administration, Funding acquisition. Aoxiang Huang: Conceptualization, Investigation. Cheng Yao, Zhengguo Tian and Tingxin Sun: Validation. Bin Zhang, Daru Chen: Supervision, Validation. Marija Bervida Mačak, Fei Gao and Samo Stanič: Data curation.

495 **Competing interests.**

The contact author has declared that none of the authors has any competing interests.

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