OUTLIER-ROBUST 4-D VARIATIONAL DATA ASSIMILATION BASED ON κ-GENERALIZED GAUSSIAN STATISTICS AND KANIADAKIS ENTROPY

by

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Original scientific paper
https://doi.org/10.2298/TSCI2602983L

In variational data assimilation, traditional methods generally presuppose that both background errors and observation errors are distributed according to the Gaussian distribution. While this assumption simplifies mathematical operations and facilitates optimization, it demonstrates notable limitations in practical applications, particularly when dealing with non-Gaussian errors and outliers. This study proposes an innovative approach to constructing the objective function based on Kaniadakis entropy and the κ-generalized Gaussian distribution. The aim of this approach is to enhance the robustness of the 4-D variational data assimilation method. The incorporation of Kaniadakis entropy into the objective function effectively characterizes heavy-tailed error distributions, thereby significantly improving the suppression of outliers and observation errors and optimizing the stability of the assimilation process. The proposed method was validated using the Lorenz-63 model. The findings indicate that the objective function founded upon the κ-generalized Gaussian distribution attains a substantial diminution in root mean square error when processing observation data that encompasses outliers. Furthermore, the assimilation results demonstrate enhanced stability and accuracy. This study provides a theoretical framework and methodological support for non-Gaussian error modeling and robust data assimilation, offering a novel perspective for data assimilation research in complex environments.

Keywords: *Kaniadakis entropy, non-Gaussian errors, robustness, data assimilation, Lorenz-63 model*

Introduction

In the domain of variational data assimilation, it is a common assumption that both background errors and observation errors follow a Gaussian distribution [1-3]. The Gaussian distribution assumption is a widely employed model to describe the statistical properties of background and observation errors due to its mathematical simplicity and ease of optimization. However, this classical assumption is known to have significant limitations in practical applications. The error distributions in real Earth systems frequently exhibit pronounced non-Gaussian characteristics [4, 5], creating a fundamental contradiction between the traditional

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Gaussian assumption and practical applications. Firstly, the probability density function (PDF) of the Gaussian distribution is characterized by symmetry and possesses thin tails [6], a property that renders it susceptible to outliers. In the context of practical observation data, the presence of outliers is inevitable, with instances of such occurrences being attributed to instrument failures or extreme weather conditions [7-9]. These outliers have the potential to exert a substantial influence on the outcomes of assimilation processes, thereby diminishing their precision and curtailing the efficacious integration of observational data within the analysis domain. Indeed, the classical framework may prove to be ill-suited even when considering a limited number of outliers. Secondly, the Gaussian distribution is inadequate in describing error distributions with heavy-tailed characteristics, such as those observed in complex terrains or weather conditions, where error distributions may exhibit asymmetry or heavy tails.

In order to overcome the limitations of the Gaussian distribution, Kaniadakis entropy, as a novel generalized entropy form, has gradually gained attention in recent years [10-13]. The property has demonstrated promising properties and application potential in fields such as statistical physics and information theory. In contrast to conventional entropy, Kaniadakis entropy has the capacity to more accurately depict non-Gaussian distributions, particularly those exhibiting heavy-tailed characteristics, by modifying the non-extensive parameter κ. By reconstructing the error terms of the objective function and generalizing the traditional quadratic cost function to a functional form based on Kaniadakis entropy, the likelihood probability of non-Gaussian errors can be quantified more accurately. This enhancement of the stability and accuracy of assimilation systems in complex scenarios confers upon them a unique advantage in the handling of non-Gaussian errors and outliers.

Variational data assimilation can be regarded as an inverse problem [14-16], and previous studies [17-19] have demonstrated that non-Gaussian criteria are more conducive to robust solutions to inverse problems. The present study proposes a novel methodology for updating the objective function in 4-D variational data assimilation, as outlined in the theory of Kaniadakis entropy. The integration of Kaniadakis entropy facilitates a more precise characterization of the non-Gaussian characteristics of errors in the objective function, thereby enhancing the robustness of assimilation algorithms against outliers. Specifically, the heavy-tailed characteristics of Kaniadakis entropy and the κ-generalized Gaussian distribution are utilized to handle observation errors and outliers. This approach not only effectively addresses non-Gaussian errors but also improves the accuracy and reliability of assimilation results to a certain extent.

The significance of this study lies in two aspects. Firstly, it extends the variational assimilation framework compatibility with non-Gaussian errors through theoretical innovation. Secondly, by addressing the practical needs of numerical weather prediction systems, it explores the potential of novel objective functions in reducing initial field errors and improving forecast timeliness.

Methods

Kaniadakis entropy and κ-generalized Gaussian distribution

Kaniadakis entropy, also referred to as κ-entropy, is a generalized entropy function that was introduced by the Italian physicist Kaniadakis [20, 21]. The proposed model extends the classical Boltzmann-gibbs entropy (Boltzmann-gibbs-Shannon entropy) by introducing a dimensionless parameter κ (satisfying $0 \le \kappa < 2/3$), thereby enabling a more flexible description of non-equilibrium systems, non-extensive systems, and statistical distributions with asymmetry or heavy-tailed characteristics. The novel κ-entropy of BGS statistics is expressed by:

$$\mathcal{S}_\kappa(p) = -\frac{1}{2\kappa}\sum_{i=1}^{N}[p^{1+\kappa}(x_i) - p^{1-\kappa}(x_i)] \tag{1}$$

In this context, $p(x)$ denotes the probability distribution, and the value of κ falls within the range [0, 2/3). Kaniadakis entropy introduces non-linearity and non-extensivity through the parameter κ, thereby extending the applicability of entropy. The disparities between Kaniadakis entropy and Shannon entropy are outlined in tab. 1.

Table 1. Differences between Kaniadakis entropy and Shannon entropy

Property	Shannon Entropy	Kaniadakis Entropy
Extensivity	Additivity	Non-extensivity (with cross-terms)
Distribution adaptability	Applicable to Gaussian distributions	Adapts to asymmetric, heavy-tailed distributions
Parameter	No adjustable parameters	Flexible control of tail properties *via* κ-parameter
Physical background	Equilibrium statistical mechanics	Non-equilibrium systems, complex systems

In the limit as the dimensionless parameter $\kappa \to 0$, Kaniadakis entropy reduces to Shannon entropy, ensuring compatibility with classical information theory.

The κ-Gaussian-based statistical framework has been proposed for error distributions applicable to various problems. Owing to its heavy-tailed nature, this framework can robustly handle outliers. The expression for the κ-Gaussian distribution is given by:

$$p_\kappa(x) = \frac{1}{Z_\kappa}\left(\sqrt{1+\kappa^2\beta_\kappa^2 x^4} - \kappa\beta_\kappa x^2\right)^{1/\kappa} \tag{2}$$

where Z_κ is the normalization constant, which is given by [22]:

$$Z_\kappa = \left(1+\frac{|\kappa|}{2}\right)\sqrt{\frac{2|\kappa|\beta_\kappa}{\pi}}\frac{\Gamma\left(\frac{1}{|2\kappa|}+\frac{1}{4}\right)}{\Gamma\left(\frac{1}{|2\kappa|}-\frac{1}{4}\right)} \tag{3}$$

where $\beta_\kappa > 0$ depends on the dimensionless parameter κ and is given by:

$$\beta_\kappa = \frac{1+|\kappa|/2}{|2\kappa|(2+3|\kappa|)}\frac{\Gamma\left(\frac{1}{|2\kappa|}-\frac{3}{4}\right)\Gamma\left(\frac{1}{|2\kappa|}-\frac{1}{4}\right)}{\Gamma\left(\frac{1}{|2\kappa|}-\frac{3}{4}\right)\Gamma\left(\frac{1}{|2\kappa|}-\frac{1}{4}\right)} \tag{4}$$

In accordance with eqs. (2) and (4), the curve of the κ-Gaussian distribution is plotted as shown in fig. 1.

Figure 1 illustrates the Gaussian probability distribution curves for different values of κ. When $\kappa \to 0$, the distribution represents the conventional Gaussian distribution. As κ increases, the peak becomes higher, and the tails of the distribution become more gradual, exhibiting power-law characteristics. When $\kappa \to 2/3$, the tails of the distribution show pronounced power-law behavior, deviating maximally from the Gaussian distribution. This makes it suitable for describing extreme events or non-linear behaviors in complex systems.

The κ-Gaussian distribution, with its tunable κ parameter, can flexibly characterize distributions ranging from the standard normal distribution to those with heavy-tailed characteristics. This property makes the κ-Gaussian distribution an attractive tool in numerical simulation and data assimilation. Based on the κ-Gaussian distribution, we derive a new objective function of variational data assimilation to replace the conventional one. Through further mathematical derivation, we obtain the gradient of this objective function, enabling effective handling of outliers during optimization. This enhances the model adaptability and robustness in extreme situations.

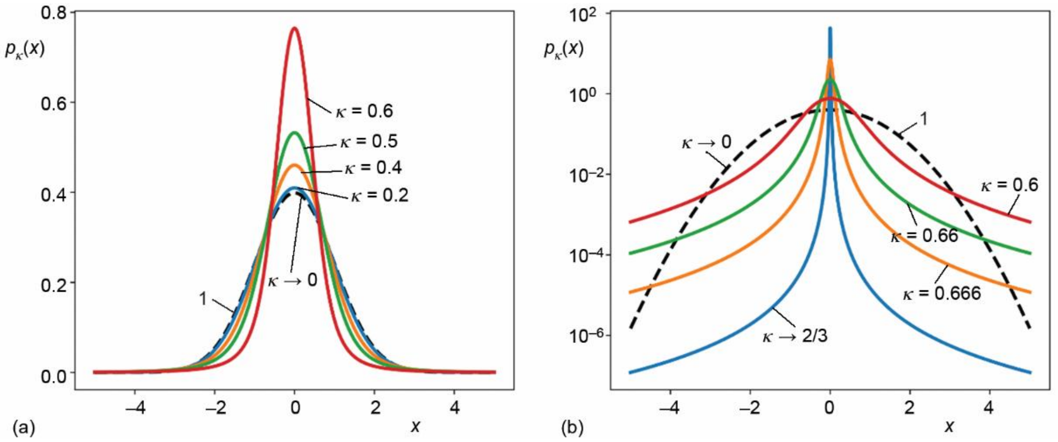

Figure 1. The κ-Gaussian probability distribution curve; black dashed line – 1 represents the conventional Gaussian distribution curve

Non-Gaussian non-linear data assimilation method based on κ-generalized Gaussian distribution

In the 4-D variational data assimilation method, if the background field errors and observation errors are assumed to follow a Gaussian distribution, the objective functional can be formulated as an optimization problem as shown in [23-25]:

$$\min J_{L_2}(x_0) = \frac{1}{2}(\mathrm{x}_0 - \mathrm{x}_b)^T \mathrm{B}^{-1}(\mathrm{x}_0 - \mathrm{x}_b) + \frac{1}{2}\int_{t_0}^{t_N} [y_\mathrm{o}(t) - y_\mathrm{m}(t)]^2 \,\mathrm{d}t \tag{5}$$

where $\frac{1}{2}[(x_0 - x_b)^T \mathrm{B}^{-1}(x_0 - x_b)]$ represents the background term, where x_b is the background field, x_0 – the initial field, and B – the background error covariance matrix. The term:

$$\frac{1}{2}\int_{t_0}^{t_N}\left[y_\text{o}(t)-y_\text{m}(t)\right]^2\,\text{d}t$$

represents the observation term, with t_0 and t_N being the start and end times of the assimilation time window, y_o being the observational data for the interval $[t_0, t_N]$, and $y_\text{m}(t)$ being the model prediction.

Since observational information is the primary source of incremental information, and the background field itself is derived from the accumulation and integration of historical observational data, we simplify the analysis by omitting the background functional term and focusing on the observational objective functional term, as shown in:

$$\min J_{L_2}(x_0)=\frac{1}{2}\int_{t_0}^{t_N}\left[y_\text{o}(t)-y_\text{m}(t)\right]^2\,\text{d}t \tag{6}$$

Equation (6) is also referred to as the minimum least squares norm (L_2-norm) form of the objective functional, which can be used to evaluate the degree of difference between model predictions and observational values. The gradient of the minimum least squares objective functional, *i. e.*, the partial derivatives with respect to the system initial state components x_{0i}, is shown in:

$$\frac{\partial J_{L_2}(\boldsymbol{x}_0)}{\partial x_{0i}}=-\int_{t_0}^{t_N}\frac{\partial y_\text{m}(t)}{\partial x_{0i}}\left[y_\text{o}(t)-y_\text{m}(t)\right]\text{d}t \tag{7}$$

Equation (6) is similar to the objective function of the 4-D variational data assimilation based on the κ-generalized Gaussian distribution, as shown in:

$$\min_{\boldsymbol{x}_0} J_\kappa(x_0)=-\frac{1}{\kappa}\int_0^T\ln\left\{\sqrt{1+\kappa^2\beta_\kappa^2[y_\text{o}(t)-y_\text{m}(t)]^4}-\kappa\beta_\kappa[y_\text{o}(t)-y_\text{m}(t)]^2\right\}\text{d}t \tag{8}$$

The partial derivative with respect to the system's initial state component x_{0i}, *i. e.*, the κ-objective function gradient, is shown in:

$$\frac{\partial J_\kappa}{\partial x_{0i}}=-\int_0^T\frac{\partial y_\text{m}(t)}{\partial x_{0i}}\frac{2\beta_\kappa[y_\text{o}(t)-y_\text{m}(t)]}{\sqrt{1+\kappa^2\beta_\kappa^2\left[y_\text{o}(t)-y_\text{m}(t)\right]^4}}\,\text{d}t \tag{9}$$

When comparing eq. (7) with eq. (9), eq. (7) corresponds to the gradient of the objective function under the traditional L2 norm (Gaussian distribution assumption). In this case, the contribution of the residual $[y_0(t) - y_\text{m}(t)]$ is linear, making it sensitive to outliers. Larger residuals lead to larger gradient contributions, allowing abnormal observations to dominate the optimization process.

Equation (9), on the other hand, corresponds to the gradient of the objective function under the κ-Gaussian distribution assumption. It introduces an adaptive weighting mechanism through the non-linear term:

$$\sqrt{1+\kappa^2\beta_\kappa^2\left[y_\text{o}(t)-y_\text{m}(t)\right]^4}$$

in the denominator. When the residual $[y_0(t) - y_\text{m}(t)]$ increases, the denominator grows much faster than the numerator, significantly reducing the gradient contribution. This mechanism automatically downweights the influence of outliers, enhancing robustness against aberrant data points.

Furthermore, the parameter κ functions as a flexible tuning mechanism. The model parameters can be calibrated to align with the characteristics of the observational data, ensuring its suitability for diverse conditions and optimization objectives. In summary, while the linear weighting mechanism in eq. (7) is vulnerable to abnormal observations, eq. (9) explicitly suppresses the impact of large residuals through a non-linear weighting function. This property renders the system more adaptable to variations in input data and system states, thereby demonstrating enhanced robustness against outliers and noise. By dynamically adjusting weights, this mechanism optimizes model or system performance, maintaining efficiency and accuracy under complex conditions, thereby enhancing the model's versatility and robustness.

Lorenz-63 model

The Lorenz-63 model, proposed by meteorologist Edward Lorenz in 1963, is a simplified 3-D non-linear dynamical system and a classic model in chaos theory and meteorology [26]. The model delineates the simplified dynamic behavior of atmospheric convection through a set of ODE, as illustrated in:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \sigma(y - x), \quad \frac{\mathrm{d}y}{\mathrm{d}t} = x(\rho - z) - y, \quad \frac{\mathrm{d}z}{\mathrm{d}t} = xy - \beta z \tag{10}$$

In the model, the variables x, y, and z represent convection intensity, the horizontal temperature gradient, and the non-linear correction of the vertical temperature profile, respectively. The parameters σ, ρ, and β represent the Prandtl number, Rayleigh number, and a geometric parameter, with typical values of $\sigma = 10$, $\rho = 28$, and $\beta = 8/3$.

The Lorenz-63 model is a paradigmatic example of deterministic chaos and the butterfly effect, where tiny initial differences lead to vastly different system states, complicating long-term prediction. As a non-linear differential equation system, it requires numerical methods for solution. In our numerical experiments using the Lorenz-63 model, we applied the fourth-order Runge-Kutta method to integrate the equations with an initial state and a time step $\mathrm{d}t = 0.01$, yielding the true state values. We assumed an initial guess $u_s = (x_s, y_s, z_s)$, then collected observations within an assimilation window of length L_{DA} and sampling interval P_{DA}. White noise with variance σ_{obs}^2 was added to the observations to generate data with a noise ratio, r.

By comparing the assimilation performance of traditional 4-DVar and κ-4-DVar under conditions with and without observational noise, we drew experimental conclusions.

Results

In this study, the assimilation integration step is set to 2800 steps, with the initial guess $u_s = (2.0,\ 3.0,\ 4.0)$. Observations are collected using an assimilation window length $L_{\mathrm{DA}} = 5$ and a sampling interval $P_{\mathrm{DA}} = 10$. The observational noise ratio is set to $r = 5\%$, with each outlier having a magnitude of 50 units. Data assimilation experiments are conducted using the Lorenz-63 model.

We compared the performance of the traditional 4-DVar method and the κ-4-DVar method on the Lorenz-63 model, both with and without observational noise. We plotted the RMSE curves of the background and analysis fields as a function of assimilation steps. The

RMSE reflects the deviation between the model and the true values. The results are shown in fig. 2.

The four subplots demonstrate the performance of two methods (4-DVar and κ-VarDA) in terms of background and analysis RMSE with and without outliers. As illustrated in figs. 2(a) and 2(b), the background and analysis RMSE comparisons for the 4-DVar method are demonstrated, while figs. 2(c) and 2(d) present a similar comparison for the κ-4-DVar method.

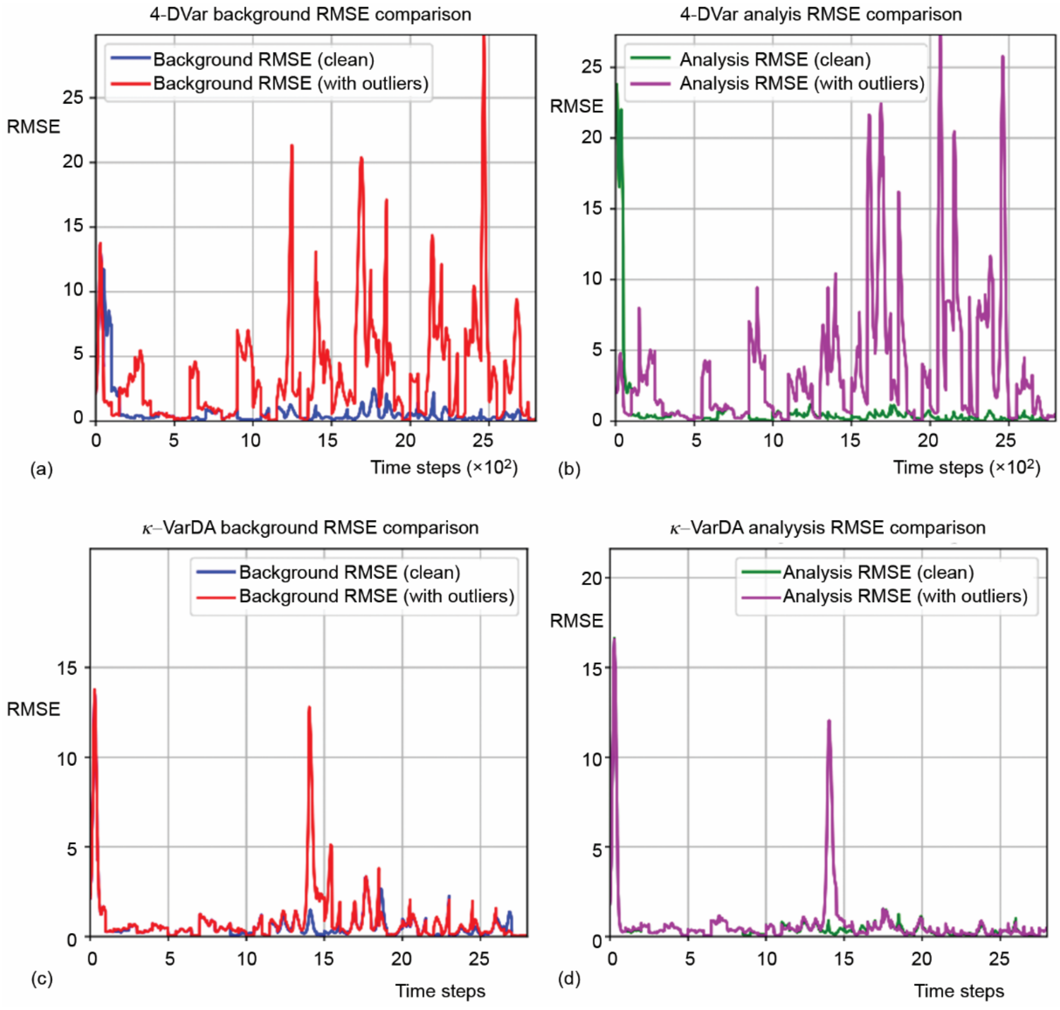

Figure 2. Comparison of the RMSE of the background field and analysis field for the traditional 4-DVar method (a), (b) and the κ-4-DVar method (c), and (d)

As illustrated in figs. 2(a) and 2(c), the blue curve signifies the background RMSE without outliers (clean), while the red curve denotes the background RMSE with outliers. As illustrated in fig. 2(a), the background RMSE maintains a low and stable level in the absence of outliers. However, when outliers are present, particularly within the time interval between 1500 and 2500 time steps, significant fluctuations are observed. This indicates that outliers exert a substantial influence on the background field estimation of 4-DVar. Conversely, as depicted in fig. 2(c), the background RMSE maintains a low and stable level, devoid of any outliers. However, it exhibits minor fluctuations between time steps 1400 and 1500, which are concomitant with the presence of outliers.

As illustrated in figs. 2(b) and (d), the green curve corresponds to the analysis RMSE excluding outliers, while the purple curve represents the analysis RMSE including outliers. It is noteworthy that both methods exhibited a consistent and stable analysis RMSE, devoid of any outliers. However, when outliers are included, the analysis RMSE of 4-DVar exhibits substantial variations between time steps 1500-2500, while the analysis RMSE of κ-4-DVar only displays negligible fluctuations between time steps 1400-1500, subsequently reaching a state of stability.

A thorough examination of the four subplots indicates that the conventional 4-DVar method demonstrates efficacy in the absence of outliers. However, it exhibits substantial variations in both background and analysis RMSE in the presence of outliers, suggesting a high degree of sensitivity to outliers. Conversely, the κ-4-DVar method exhibits low and stable RMSE, both with and without outliers, thereby demonstrating enhanced robustness. Consequently, κ-VarDA demonstrates enhanced stability and robustness in the handling of outliers, rendering it well-suited for scenarios characterized by frequent occurrences of outliers.

Discussion and summary

This study addresses the limitations of traditional 4-DVar in handling non-Gaussian errors and outliers by proposing an outlier-resistant 4-D variational assimilation method (κ-VarDA) based on Kaniadakis entropy and κ-generalized Gaussian distribution. The incorporation of Kaniadakis entropy has been demonstrated to augment the efficacy of the objective function in accurately representing heavy-tailed error distributions. This enhancement is achieved through the implementation of a non-linear weighting mechanism, which effectively suppresses interference from outliers.

Numerical experiments employing the Lorenz-63 model have demonstrated that κ-VarDA significantly reduces background and analysis RMSE in the presence of outliers. This finding suggests that κ-VarDA demonstrates enhanced robustness and stability. Theoretically, this study innovates by proposing a Kaniadakis entropy-based 4-DVar objective function, extending the traditional Gaussian assumption to effectively handle non-Gaussian errors. Methodologically, it enhances the efficacy of assimilation algorithms by dynamically adjusting residual contributions through the implementation of non-linear weighting. The Lorenz-63 experiments substantiate the efficacy of the method in complex non-linear systems, particularly in preserving stability and accuracy in the presence of outliers. While traditional 4-DVar performs adequately in the absence of outliers, it demonstrates substantial RMSE fluctuations in the presence of outliers, thereby signifying its sensitivity. Conversely, κ-VarDA exhibits diminished variability in its RMSE fluctuations and expedited stabilization, thereby emphasizing its resilience and reliability.

Notwithstanding these advantages, the applicability of κ-VarDA in higher-dimensional systems necessitates further verification, and the optimization of the κ parameter for different data characteristics remains a subject of active research. Subsequent studies may involve the implementation of this method within authentic numerical weather prediction systems.

In conclusion, κ-VarDA offers a novel framework for non-Gaussian error modeling and robust data assimilation, demonstrating notable resilience in handling outliers and providing a promising tool for numerical weather prediction and data assimilation. Subsequent research endeavors may further refine this method and investigate its broader applications.

Acknowledgment

We sincerely appreciate the contributions of everyone who supported and participated in this research.

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Paper submitted: December 30, 2024
Paper revised: April 7, 2025
Paper accepted: April 17, 2025

2026 Published by the Vinča Institute of Nuclear Sciences, Belgrade, Serbia.
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