Identifying large-scale atmospheric patterns that modulate extremes in local-scale variables such as precipitation has the potential to improve long-term climate projections as well as extended-range forecasting skill. This paper proposes a novel probabilistic machine learning method, RMM-VAE, based on a variational autoencoder architecture for identifying weather regimes targeted to a local-scale impact variable. The new method is compared to three existing methods in the task of identifying robust weather regimes that are predictive of precipitation over Morocco while capturing the full phase space of atmospheric dynamics over the Mediterranean. RMM-VAE performs well across these different objectives, outperforming linear methods in reconstructing the full phase space and predicting the target variable, highlighting the potential benefit of applying the method to various climate applications such as downscaling and extended-range forecasting.
dynamic and thermodynamic components of climate change for extreme event attribution, to
downscale or bias-adjust climate models [4]–[6], and to quantify the role of atmospheric internal
variability in observed trends [7], [8]. Moreover, weather regimes have been shown to improve the
usability and skill of forecasts at sub-seasonal-to-seasonal timescales [9]–[12].

To identify weather regimes, a combination of dimensionality reduction and clustering is commonly
applied to gridded geopotential height or sea level pressure data of the region of interest. Following
[13], principal component analysis (PCA) and k-means have established themselves as common
choices for dimensionality reduction and clustering respectively, although various other linear
statistical methods have been studied in the field [3]. Recent publications have also explored non-

While the relationship between weather regimes and extremes in local impact variables (e.g. extreme
precipitation) is a key motivation for their investigation, there are no comprehensive methods
available for identifying probabilistic weather regimes targeted to a specific impact variable, without
compromising regime completeness or persistence [16]–[18]. By 'targeting' weather regimes, we
mean identifying patterns in the high-dimensional space of atmospheric dynamics that are
particularly predictive of the local-scale variable in question while still capturing the full dynamics
of the atmospheric phase space. As this last point is particularly relevant for extending the forecast
range of the impact variable through the extended range predictability of the patterns, building a
purely predictive ML model of the impact variable is not useful in this context.

This paper presents a novel probabilistic machine learning method for identifying weather regimes
that captures the full phase space of atmospheric dynamics in a reduced space while providing
enhanced predictability of a local-scale impact variable. The proposed method, which we call RMM-
VAE (Regression Mixture Model Variational Autoencoder), integrates both targeted dimensionality
reduction using a variational autoencoder (VAE), and probabilistic clustering using a mixture model
(MM) into one coherent statistical model, extending previous machine learning architectures
reported in [19], abbreviated R-VAE (Regression - VAE) here, that incorporate a co-variate into the
dimensionality reduction step of a VAE model, without combining it with a clustering.

To demonstrate the performance of the RMM-VAE method, it is compared to existing methods in
the task of identifying weather regimes targeted to precipitation over Morocco, which serves as our
target variable here. To evaluate the performance of RMM-VAE, we compare our method to two
established approaches (PCA + k-means, and CCA + k-means), as well as the R-VAE method
combined with k-means clustering (R-VAE + k-means). The performance of all methods is assessed
on three possible objectives of targeted clustering: reconstruction of the input space, persistent and
well-separated clusters, and predictive skill with respect to the target variable.

2 Proposed RMM-VAE method

Figure 1 (left side) shows a schematic of the proposed method RMM-VAE. We introduce a scalar
co-variate t into the inference model, extending the architecture developed by [19] by conditioning
the dimensionality reduction on a probabilistic cluster assignment [20], [21]. Using the graphical
model shown in Figure 1 (right side), the joint probability distribution of the model is obtained and
the loss function derived using Bayesian Variational Inference [22] (details in appendix A).
Figure 1: Left side: Schematic diagram of the RMM-VAE method which combines a regression VAE (R-VAE, based on [19]) with probabilistic clustering using mixture models (MM). Right side: RMM-VAE model written as a probabilistic graphical model in plate notation to facilitate the derivation of the loss function using Bayesian variational inference. $x$ represents the high-dimensional input data, $z$ the latent space with prior $\phi_k$ depending on the cluster assignment, as well as parameters $\theta$ depending on the cluster assignment, $t$ the scalar target variable, with probabilistic cluster assignment $c$ with prior $\pi_k$. In both panels, dashed lines indicate the inference model and solid lines the generative model.

3 Experiments

The performance of RMM-VAE is compared to two more established linear statistical methods, namely PCA and canonical correlation analysis (CCA), respectively combined with k-means clustering. The performance of the integrated, probabilistic clustering implemented in RMM-VAE is also compared with a version that separates targeted dimensionality reduction in an architecture based on [19] with a separate k-means clustering step (R-VAE + k-means). A description of PCA, CCA, k-means and a standard VAE architecture can be found in [23], and a derivation of the R-VAE method in [19].

Table 1 provides an overview of the compared methods along with relevant hyperparameters. A 10-dimensional latent space was implemented for all the methods, and cluster numbers between 4 and 10 were investigated. For both VAE methods, the inclusion of a hyperparameter $\beta$ [24] which changes the weight of the reconstruction term in the loss function was investigated (v1 and v2).

Table 1: Overview of the methods applied to the identification of weather regimes and associated parameter choices

<table>
<thead>
<tr>
<th>Abbr.</th>
<th>Method</th>
<th>$\beta$</th>
<th>Precipitation data</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCA</td>
<td>PCA + k-means</td>
<td>-</td>
<td>Full daily precipitation field at 0.25° resolution</td>
</tr>
<tr>
<td>CCA</td>
<td>CCA + k-means</td>
<td>-</td>
<td>Spatially averaged daily precipitation (scalar)</td>
</tr>
<tr>
<td>R-VAE v1</td>
<td>R-VAE + k-means</td>
<td>1</td>
<td>&quot; - &quot;</td>
</tr>
<tr>
<td>R-VAE v2</td>
<td>R-VAE + k-means</td>
<td>0.1</td>
<td>&quot; - &quot;</td>
</tr>
<tr>
<td>RMM-VAE v1</td>
<td>RMM-VAE</td>
<td>1</td>
<td>&quot; - &quot;</td>
</tr>
<tr>
<td>RMM-VAE v2</td>
<td>RMM-VAE</td>
<td>0.5</td>
<td>&quot; - &quot;</td>
</tr>
</tbody>
</table>

To analyze weather regimes over the Mediterranean region (latitude: 25°N — 50°N; longitude: 10°W — 45°E) applying these methods, geopotential height at 500hPa ($z_{500}$) from ERA5 reanalysis data, 1940 — 2022 was using as input data $x$. The data was standardized by subtracting the daily mean and dividing by the standard deviation over the considered time period. ERA5 reanalysis data of daily total precipitation data in a region over Morocco (latitude: 30°N — 36°N; longitude: 11°W — 0°E) over the same time period were used as the target variable. Precipitation data was normalized by applying a Box-Cox transformation at each grid cell. A three-day average of daily
total precipitation around each day was taken to mirror methodologies previously applied in the study of precipitation extremes over the Mediterranean [25]. The same was applied to z500 data to match the two datasets.

4 Results

Analyzing the latent space of the four methods shown in Figure 2 (top row), we find that both of the targeted VAE methods, RMM-VAE and R-VAE + k-means, disentangle the dimension in the latent space associated with the target variable, which is in line with the findings presented by [19] for the R-VAE method. However, what is interesting is that the cluster assignment (Figure 2, bottom row) differs between the two methods: R-VAE + k-means, which carries out the cluster assignment in a separate step, identifies the clusters in bands along the dimension associated with the target variable. In contrast, RMM-VAE, which integrates a probabilistic cluster assignment with the targeted dimensionality reduction, shows less organization of the clusters with respect to the target variable.

The performance of the dimensionality reduction component was analyzed by computing the root mean square error between the reconstructed space and the original input data. We find that both VAE methods outperform the two linear statistical methods, and that decreasing the weight of the reconstruction loss term ($\beta < 1$) in the v2 versions increases the reconstruction loss. When investigating the reconstruction of individual data points, we find that decreasing the $\beta$-parameter focuses the dimensionality reduction on the region immediately surrounding Morocco. The figures to support these results are shown in the supplementary appendix B.

![Figure 2: Visualization of the 10-dimensional latent space reduced to two dimensions using t-distributed stochastic nearest-neighbor embedding (t-SNE). Different values of perplexity were tested and perplexity=10 was chosen as it shows representative results. Embedded data points are colored first according to the target variable, total mean precipitation (top row) with darker colors referring to stronger precipitation, and then according to the cluster they are subsequently assigned to in the corresponding clustering method (bottom row).](image)

Investigating the predictive performance of the clusters using the Ranked Probability Skill Score (supporting derivation and figures shown in supplementary appendix C), we find that both VAE methods outperform both CCA and PCA up to a cluster number of 9, which shows the potential of targeting weather regimes to a local impact variable by introducing a co-variate to a VAE architecture. While the R-VAE + k-means method outperforms RMM-VAE in terms of predictive skill, the R-VAE + k-means clusters are less persistent and separable compared to RMM-VAE, assessed using the silhouette score. In both methods, the v2 versions which deprioritize the reconstruction term in the loss function ($\beta < 1$) identify clusters with higher predictive skill but lower cluster persistence and separability, compared to the respective v1 versions ($\beta = 1$). This finding highlights the trade-off between the predictive skill of weather regimes for a given target variable, which would be maximized in a purely predictive model, and identifying robust clusters, which is important for using the weather regimes for extended-range prediction and for linking regional extremes to global patterns of climate change.
5 Conclusion

The paper introduced a novel machine learning method, RMM-VAE, for the identification of weather regimes with respect to a scalar target variable. The novelty of this method lies in developing an architecture that combines non-linear, probabilistic, and targeted dimensionality reduction with probabilistic clustering using mixture models in a coherent Bayesian probabilistic framework. The new method performs well across all the different objectives analyzed, outperforming the linear methods in reconstructing the full phase space and in predicting the target variable. Compared to the other machine learning method, R-VAE + k-means, the proposed RMM-VAE method loses in predictive skill but identifies more persistent and separable clusters, which is relevant for various climate applications such as extended-range forecasting or the downscaling of climate models, highlighting the potential benefit of applying the RMM-VAE method to these use-cases. In future work, we are planning to analyze the dynamical processes captured by the targeted clusters and extend the architecture to identify joint clusters between two high-dimensional spaces.
Acknowledgments

Include only in final version.

References


Supplementary Appendices

A - RMM-VAE method: loss function

The assumptions of the model can be expressed in a probabilistic graphical model and the joint probability distributions of the model can then be written as:

\[ p_\theta(x, z, t, c^k) = p_\theta(x|z)p(z|t)p(t)p(z|c^k)p(c^k) \]

\[ q_\phi(z, t, c^k|x) = q_\phi(x|z)q_\phi(t|x)q_\phi(c^k|x) \]

The loss function can then be derived as:

\[ \mathcal{L}(x) = -D_{KL}(q_\phi(z, c, t|x) \parallel p_\theta(x, z, t, c)) \]

\[ = \sum_k q_\phi(c^k|x) \left[ E_{q_\phi(z|x)} \left[ \log(p_\theta(x|z)) \right] - E_{q_\phi(t|x)} \left[ D_{KL}(q_\phi(z|x) \parallel p(z|t)) \right] \right] \]

\[ - D_{KL}(q_\phi(t|x) \parallel p(t)) - D_{KL}(q_\phi(z|x) \parallel p(z|c^k)) \]

\[ - D_{KL}(q_\phi(c^k|x) \parallel p(c^k)). \]

B - Additional figures - reconstruction loss

Figure 3: Distribution of root mean squared error (RMSE) between original input data and data reconstructed from dimensionality-reduced space over all data points, for the different methods.

Figure 4: Gridded and normalized z500 anomalies, as detailed in section 2, on an example day 1940-01-04, showing the original data on the left and the reconstructions using different methods on the right.

C - Assessment of predictive skill

To evaluate the informativeness of the weather regimes with respect to the target variable, and in particular their utility for extended-range forecasting, we analyze the Ranked Probability Skill Score (RPSS) which is widely used in forecast evaluation. The RPS is defined as \( RPS = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{m} \left( \delta_{i,j} - p_i \right)^2 = -\frac{1}{N} \sum_{i=1}^{N} (1 - 2p_i + \sum_{j=1}^{m} p_j^2) \), and the score (RPSS) calculated with respect to a reference forecast, chosen here to be the climatology over the entire period.
\[ \text{RPSS} = 1 - \frac{\text{RPS}_{\text{forecast}}}{\text{RPS}_{\text{climatology}}} \], with \( m \) forecast categories and \( N \) timesteps. \( \delta_{i,n,j} \) is the Kronecker delta and equals 1 if the observation \( i \) at timestep \( n \) corresponds to category \( j \), and 0 otherwise. The RPSS is a strictly proper scoring rule to measure the accuracy of a probabilistic prediction of mutually exclusive discrete outcomes [26]. A RPSS of 1 indicates a perfect forecast while low values indicate little, or no skill compared to the reference forecast. Here, we construct a forecast of the target variable given the occurrence of a weather regime and the conditional probability of the target variable given that weather regime: each discrete target is forecast with a probability corresponding to the probability of the weather regime at this given day, multiplied by the climatological conditional probability of the target given the weather regime.

**Figure 5**: Ranked Probability Skill Score for forecast of mean precipitation over Morocco given weather regimes at zero lead time for different numbers of weather regimes. a) Skill score for binary forecast above or below 95th percentile and c) Skill score for forecast of the tercile of the precipitation distribution. For probabilistic clustering, this skill score is computed using the most likely cluster at the given data point.