# Reconstructing balloon-observed gravity wave momentum fluxes using machine learning and input from ERA5

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# Key Points:

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12	•	Eight superpressure balloons from the Strateole 2 mission provide observations
13		for accurate gravity wave momentum flux estimation
14	•	Three machine learning methods are employed to probe the relationship between
15		the gravity wave momentum fluxes and ERA5's large-scale flow
16	•	The most informative large-scale inputs are provided, along with a discussion of
17		the successes and challenges of machine learning methods

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## 18 Abstract

Global atmospheric models rely on parameterizations to capture the effects of gravity 19 waves (GWs) on middle atmosphere circulation. As they propagate upwards from the 20 troposphere, the momentum fluxes associated with these waves represent a crucial yet 21 insufficiently constrained component. The present study employs three tree-based en-22 semble machine learning (ML) techniques to probe the relationship between large-scale 23 flow and small-scale GWs within the tropical lower stratosphere. The measurements col-24 lected by eight superpressure balloons from the Strateole 2 campaign, comprising a cu-25 mulative observation period of 680 days, provide valuable estimates of the gravity wave 26 momentum fluxes (GWMFs). Multiple explanatory variables, including total precipita-27 tion, wind, and temperature, were interpolated from the ERA5 reanalysis at each bal-28 loon's location. The ML methods are trained on data from seven balloons and subse-29 quently utilized to estimate reference GWMFs of the remaining balloon. We observed 30 that parts of the GW signal are successfully reconstructed, with correlations typically 31 around 0.54 and exceeding 0.70 for certain balloons. The models show significantly dif-32 ferent performances from one balloon to another, whereas they show rather compara-33 ble performances for any given balloon. In other words, limitations from training data 34 are a stronger constraint than the choice of the ML method. The most informative in-35 puts generally include precipitation and winds near the balloons' level. However, differ-36 ent models highlight different informative variables, making physical interpretation un-37 certain. This study also discusses potential limitations, including the intermittent na-38 ture of GWMFs and data scarcity, providing insights into the challenges and opportu-30 nities for advancing our understanding of these atmospheric phenomena. 40

## <sup>41</sup> Plain Language Summary

Part of the atmosphere's large-scale circulation results from motions that are not 42 resolved, or partly resolved, by weather or climate models. These include internal grav-43 ity waves, with horizontal scales from a few to hundreds of kilometers. The main sources 44 occur in the troposphere, such as flow over mountains and cloud development. Their three-45 dimensional propagation induces major aggregated impacts in the stratosphere and meso-46 sphere, forcing key aspects of the circulation. This forcing is accounted for in climate mod-47 els by 'parameterizations', that mimics the effect of the unresolved waves based on the 48 large-scale, resolved flow. These parameterizations necessarily retain crude approxima-49 tions and introduce significant uncertainty in the models. For GWs, sources are a ma-50 jor uncertainty. This study makes use of the high-altitude balloon campaign Strateole 51 2 (Oct. 2019-Feb. 2020). Eight balloons circled Earth at heights around 18 to 20 km, 52 providing unique observations of the GWs. These are used as targets for machine learn-53 ing (ML) methods that take as inputs the information from outputs of a numerical weather 54 prediction model describing the large-scale flow. The successes and difficulties of ML pro-55 vide insights which can guide improvements of parameterizations, such as the most in-56 formative large-scale variables for estimating the unresolved waves. 57

## <sup>58</sup> 1 Introduction

Climate models and Numerical Weather Prediction models resolve a widening range 59 of atmospheric processes as computing power increases, enabling finer spatial resolution. 60 Subgrid-scale processes persist nonetheless, and efforts to improve and constrain them 61 better are essential. Internal gravity waves constitute one of these subgrid-scale processes, 62 with important implications for the circulation and variability of the middle atmosphere 63 (Fritts & Alexander, 2003). Motivations for improved modeling of the stratosphere in-64 cludes climate (e.g. Solomon et al. (2010); Kremser et al. (2016)) but also predictabil-65 ity on shorter time scales (F. Vitart and A.W. Robertson, 2018; Butchart, 2022). 66

Gravity waves occur on scales ranging from a few to several hundreds of kilome-67 ters. An important effect stems from their vertical propagation: gravity waves are re-68 sponsible for vertical transfers of momentum from lower layers (troposphere: denser and 69 with more gravity wave sources) to upper layers (stratosphere and beyond), where they 70 constitute an essential driver of the overall circulation (Fritts & Alexander, 2003). A sig-71 nificant part of the spectrum of gravity waves has been and remains unresolved in global 72 models, requiring these effects to be represented by parameterizations (Kim et al., 2003). 73 Models display sensitivity to these, calling for coordinated efforts to better constrain these 74 parameterizations from both observations and high-resolution modeling (Alexander et 75 al., 2010). 76

A global comparison of observed, resolved and parameterized gravity wave momen-77 tum fluxes was carried out by Geller et al. (2013), highlighting significant discrepancies. 78 Although GWs parameterizations are now used routinely in climate models, their val-79 idation against in situ observations remains a challenge. There exist global observations 80 derived from satellite observations (e.g. Ern et al. (2018)), but there are limitations on 81 the wavelengths that can be observed, and significant assumptions are needed to indi-82 rectly deduce important quantities like the momentum fluxes from temperature fluctu-83 ations, using polarization relations (Alexander et al., 2010; Ern et al., 2014). For these 84 reasons superpressure balloons have been highlighted as a valuable and accurate source 85 of information on gravity wave momentum fluxes (Geller et al., 2013). A downside of su-86 perpressure balloon observations is their very sparse sampling of the lower stratosphere: 87 despite a broad coverage of the Southern Ocean (Jewtoukoff et al., 2015) and of the equa-88 torial belt (Corcos et al., 2021), each balloon flight provides only local information: one 89 time series along its trajectory. 90

There are fundamental difficulties in validating parameterizations of gravity waves: 91 the purpose of a parameterization is to provide the forcing to the large-scale which is miss-92 ing because of unresolved processes. Ideally, one would wish to know what this forcing 03 should be and validate this outcome of parameterizations. Unfortunately, this forcing cannot be directly observed. Validating parameterizations by the realism of the clima-95 tology and variability of the atmospheric circulation in global models constitutes a first 96 step, but is not a severe test and allows for compensating errors between parameterized 97 processes (Plougonven et al., 2020). More stringent tests involve comparisons to obser-98 vations (de la Camara et al., 2014; Trinh et al., 2016). Recently, direct comparisons be-99 tween observed and parameterized gravity waves have been carried out on the scale of 100 daily variations rather than at the level of general statistical characteristics (Lott et al., 101 2023). The large-scale environment was described using the ERA5 reanalyses (Hersbach 102 et al., 2020), providing the background fields necessary to emulate the parameterization 103 of convectively generated waves of Lott & Guez (2013), which is the parameterization 104 used in the climate model of IPSL (Institut Pierre Simon Laplace, Boucher et al. (2020)). 105 The comparison was quite encouraging, with the gravity wave momentum fluxes hav-106 ing the right order of magnitude, and an appropriate intermittency. 107

An essential aspect, and fundamental issue, to keep in mind when comparing ob-108 served and modeled gravity wave momentum fluxes is their strong intermittency: in time 109 series of GWMF, one commonly finds short, intense peaks corresponding to a strong grav-110 ity wave event, surrounded by considerably weaker values. This has been highlighted in 111 the long 'tail' of the Probability Density Function (PDF) of the GWMF (Alexander et 112 al., 2010; Hertzog et al., 2012), and quantified in simulations and observations (Plougonven 113 et al., 2013; Wright et al., 2013; Ern et al., 2022). This intermittency further contributes 114 to making the parameterization of gravity waves a challenging task. 115

For the improvement of parameterizations in general (not only those of gravity waves), machine learning methods provide an array of possibilities. These have been explored in different directions:

- Machine learning can enable the emulation of parameterizations, leading to sig-119 nificant computational time savings (Chantry et al., 2021; de Burgh-Day & Leeuwen-120 burg, 2023). 121 • Machine learning can help to capture the relationship between large-scale fields 122 and the unresolved process, as illustrated in the case of convection by Gentine et 123 al. (2018). For exploration, the dataset used as the truth came from a higher-resolution 124 simulation, not from observations; obtaining observationally based knowledge of 125 the effects to be parameterized remains a major challenge. 126 • Machine learning can be used to explore the relationship between the large-scale 127 flow and the resulting small-scale waves, as has been done for orographic waves 128 over Northern Japan (Matsuoka et al., 2020). Again, both the target and the in-129 puts are modelled fields, but at different resolutions. 130 • As a precursor to a data-driven parameterization that would have learned from 131 observations, a machine learning-based emulator of a parameterization for grav-132
- ity waves has been used in a climate model, including under climate change con ditions (Espinosa et al., 2022).

The purpose and scope of the present study is to probe the relationship between 135 the large-scale flow and gravity waves in the Tropics, using machine learning approaches 136 to address fundamental issues: what fraction of the GWMF can be determined from knowl-137 edge of the large-scale flow, and what fraction remains as *stochastic*? Which large-scale 138 variables are most informative, and do they match with our common understanding of 139 underlying gravity wave parameterizations? The present study belongs to the third cat-140 egory outlined above for the uses of machine learning (the purpose is *not* to produce a 141 new parameterization, nor to emulate an existing one). With similar goals, Amiramjadi 142 et al. (2023) used machine learning methods to probe the relationship between the large-143 scale flow and gravity waves, for non-orographic waves in the mid-latitudes and using 144 waves resolved in a reanalysis as a target. In contrast, the present study aims at observed 145 momentum fluxes in the Tropics, where the Strateole 2 campaigns provide a wealth of 146 new observations (Haase et al., 2018; Corcos et al., 2021). 147

The paper is organized as follows: Section 2.1 provides an overview of the data and ML algorithms used in this study. Section 3 presents the performances of ML methods in reconstructing the reference GMWFs. Section 4 discusses the factors that influence the performances and addresses the limitations of ML methods. Finally, Section 5 concludes the study with key takeaways and future directions.

#### <sup>153</sup> 2 Data and methodology

## 2.1 Data

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We use in situ observations collected from eight constant-level balloon flights (al-155 titude between 18.5 and 20km) during the Strateole-2 mission from November 2019 to 156 February 2020 (Corcos et al., 2021). As in Corcos et al. (2021), momentum fluxes (MFs) 157 were computed from raw balloon measurements following the procedure described in Vin-158 cent and Hertzog (2014). Essentially, the pressure and horizontal wind time series are 159 first projected in the time-frequency domain thanks to a continuous wavelet transform 160 (Torrence and Compo, 1998). The pressure observations inform on the vertical displace-161 ments of the balloon, which are related to those of air parcels, assuming that the bal-162 loon behaves as a perfect isopycnic tracer. The time-frequency MF decomposition is then 163 derived from the wavelet cross-spectrum of the horizontal winds and air-parcel vertical 164 displacements. Segments polluted by non-geophysical artifacts (e.g. depressurization events) 165 are discarded. 166

For our analysis, and following Corcos et al. (2021), we considered gravity wave MFs integrated over two frequency bands: a high-frequency (HF) band (i.e. short pe-

riods, ranging from 15 minutes to 1 hour) and wide-frequency (WF) band (i.e., long pe-169 riods, ranging from 15 minutes to 1 day). For the sake of readability, in all that follows 170 we focus on the HF band, unless explicitly stated. Additionally, we also differentiate be-171 tween eastward-propagating waves that yield positive MF in the zonal direction (east-172 ward) and westward-propagating waves that produce negative MF (westward). We use 173 these MFs as a reference for the true target MFs. Then, we pair them with large-scale 174 flow input information from ERA5, such as wind velocity (u and v), temperature (temp), 175 total precipitation (tp) and logarithm of surface pressure (lnsp). These fields are retrieved 176 for each balloon, from fields at a resolution of  $1^{\circ} \times 1^{\circ}$ , at the grid point closest to the 177 balloon position. Additionally, the same input variables have been retrieved in the vicin-178 ity of a 5 by 5 horizontal square centered on the grid point closest to the balloon; in the 179 present study, only total precipitation in this extended area around the balloon will be 180 used. In the vertical, the ECMWF model comprises a total of 137 levels. Four levels are 181 retained in the present study, to succinctly describe the vertical wind profile from the 182 surface to balloon flight level (see Table 1). 183

The inputs and the targets are interpolated and averaged into 1-hour time resolution. The three ML models are trained using 3-hour time averaging data, and their performance will be evaluated based on daily averaging time resolution, as presented in Lott et al. (2023). Table 1 presents the finalized large-scale flow variables utilized for training ML models.

## 2.2 Methodology

In this study, three tree-based ensemble ML methods are considered: random forest (RF) introduced in Breiman (2001), extremely randomized trees also known as extratrees (ET) by Geurts et al. (2006), and Adaptive Boosting or Adaboost regressors by Freund & Schapire (1997). These algorithms construct multiple decision trees, and the final prediction is determined by aggregating the individual decision tree predictions.

It should be noted that other methods, such as deep neural networks, as well as other types of networks including convolutional and recurrent neural networks, have also been implemented. However, the performances of these methods are not comparable to the presented tree-based algorithms, as these models typically require a large number of observations to achieve comparable results. The limitations and concerns regarding the models, the large-scale input variables, the target observations, and the nature of the relation between the large-scale and small-scale flow will be discussed later in Section 4.3.

## 202 2.2.1 Decision tree

The decision tree algorithm (Breiman et al., 1984) is the foundational building block of the primary ML methods used for our predictions. They are widely used for nonlinear prediction problems due to their efficiency and interpretability. To construct a decision tree, the training data is recursively partitioned into small hyperrectangular regions of the forms  $R_1 = \{X \leq \alpha\}$  and  $R_2 = \{X > \alpha\}$  for some ERA5 input variable X (wind velocity or precipitation, for instance) and threshold  $\alpha$ . At each step, we recursively split the input space into hyperrectangular regions that are as pure as possible. Purity refers to the homogeneity of the training target y (GWMF) within each region, and Total Within Sum of Squares (TWSS) is utilized as the impurity measure in this study. Specifically, a split is performed at any input variable X at threshold  $\alpha$  if it minimizes the following TWSS criterion:

$$\sum_{y \text{ of } R_1} (y - \mu_1)^2 + \sum_{y \text{ of } R_2} (y - \mu_2)^2,$$

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•  $R_1$  and  $R_2$  are the left and right regions of the split

•  $\mu_1$  and  $\mu_2$  are the average targets within region  $R_1$  and  $R_2$  respectively.

Any new observation must belong to one of these regions, and its prediction is determined by averaging the target values of all the neighboring observations within that block. Constructing an optimal tree is generally challenging, and the tree's structure, such as its depth and the minimum size of regions allowed to split, are hyperparameters that need to be optimized. Figure 1 below provides an example of a simple decision tree trained on 100 observations of precipitation and zonal wind velocity to predict absolute GWMF.



**Figure 1.** An example of a simple decision tree built using precipitation and wind velocity to predict absolute GWMF. The left side is the partition cell representation of the tree on the right side. The data points are colored according to the value of their target GWMF.

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## 2.2.2 Random forest

Random forest (RF) is a powerful ensemble learning method that aims at minimiz-214 ing variance across a collection of decision trees by averaging their predictions (Breiman, 215 2001). The term 'random' signifies the deliberate characteristic of constructing individ-216 ual trees using different bootstrap samples (sampling observations with replacement) and 217 exploring only a small, randomly selected, subset of the complete input features. This 218 approach effectively decorrelates the individual trees, resulting in a reduction of predic-219 tion variance. Additionally, the construction of each individual tree using only a small 220 subset of input features enables random forest to handle high-dimensional data effectively. 221 The key hyperparameters in a random forest are the number of trees, tree complexity, 222 and the number of randomly selected features used in building the individual trees. Fine-223 tuning these hyperparameters is essential to optimize the performance of the method. 224

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## 2.2.3 Extremely randomized trees

Extremely randomized trees or Extra-trees (ET) operates similarly to RF approach, with the distinction that each tree is constructed using the complete training data, and each split is performed at *random values* using a *random subset* of input features (Geurts et al., 2006). This results in a high degree of independence among the trees and can occasionally yield remarkable results compared to the random forest method.

## 2.2.4 Adaptive boosting

Adaptive boosting (Adaboost) combines weak learners to create a strong predictive model (Freund & Schapire, 1997). Weak learners refer to predictive models that per-

form slightly better than random guesses, and simple decision trees with only a few splits 234 (stumps) are used as weak learners in this study. During each iteration, Adaboost com-235 bines an individual stump by using a weighted sum, where the weight assigned to the 236 current stump is determined based on its overall performance in predicting the target 237 variable. Additionally, the weights associated with the individual training data points 238 are adjusted manually based on their prediction accuracy, giving more attention or weight 239 to points with poor predictions in the next iteration. Adaboost is well known for its abil-240 ity to mitigate overfitting (Rätsch et al., 2001) and has achieved significant success in 241 various prediction challenges (see, for example, Benjamin Bossan (2015) and ZEWEICHU 242 (2019)).243

#### 244 2.2.5 K-fold cross validation

K-fold cross-validation is the most commonly used model selection technique in ma-245 chine learning. It involves dividing the training data into K parts or folds, namely  $F_1, \ldots, F_K$ , 246 then a model is trained on K-1 folds, and it is tested on the remaining one. This pro-247 cess is repeated K times and the final performance is the average performance over all 248 the K different testing folds. In this study, K-fold cross-validation is used to prevent over-249 fitting and to select the best possible hyperparameters of each ensemble method. More 250 precisely, if  $f_{\theta}$  is the considered method (random forest, for example) with a hyperpa-251 rameter  $\theta \in \Theta$ , then the optimal hyperparameter  $\theta^*$  is defined by, 252

$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmin}} \frac{1}{K} \sum_{k=1}^{K} \sum_{(x_i, y_i) \in F_k} (f_{\theta}(x_i) - y_i)^2.$$
(1)

In our study,  $\theta$  consists of the depth of the decision trees (maximum number of splits performed from the root node to the leaves), the size of random subsets of the ERA5 input features to be considered when building individual trees, and the number of decision trees used in each ensemble learning method. All these keys are tuned using 10-fold cross-validation.

We first train ML models with an extensive set of ERA5 inputs. Subsequently, we refine these inputs to a more manageable subset (see Table 1 below) using importance feature scores, which will be described in Section 3. Moreover, in order to reduce the influence of extreme values in the target and increase its normality, the Box-Cox transformation (Box & Cox, 1964) is performed on the GWMF y to obtain the transformed target  $\tilde{y}$ :

$$\tilde{y} = \frac{y^{\lambda} - 1}{\lambda}.$$

In the experiment, the exponent  $\lambda = 0.6$  is chosen based on the performance of models trained on the corresponding transformed target data. The predictions given by ML models are then reverted using the inverse transformation:

$$y = (1 + \lambda \tilde{y})^{1/\lambda}$$

Moreover, to predict any GWMFs (absolute, eastward, or westward GWMFs of HF or WF case) of any given balloon, the ML models are trained using data from the seven other balloons. The models are fine-tuned using a 10-fold cross-validation method to optimize their performances.

Finally, the resolutions used for the data (see Section 2.1) reflect the phenomena we aim to estimate. From large-scale information as described from reanalyses at a resolution of  $1^{\circ} \times 1^{\circ}$  and hourly in time, it is only reasonable to estimate GWMFs averaged over a comparable timescale (one hour). As the balloons drift at velocities typically ten to twenty m.s<sup>-1</sup>, this corresponds to sampling over a spatial area of several tens of kilometers. The final choice for the specific setting used has been also guided by the motivation to make comparison with the results of Lott et al. (2023) possible.

The targeted gravity waves, as observed by the balloons, cover the whole range of 270 intrinsic frequencies. The high frequency band (HF, see Section 2.1) may a priori be more 271 difficult to predict from ML because it is expected to be more intermittent (Corcos et 272 al., 2021), so that sampling will be a more severe issue than for the WF band. On the 273 other hand, higher frequency waves propagate more vertically and are shorter-lived, both 274 275 factors contributing to a stronger causal relationship between local conditions below the balloons and observed gravity at balloon level. As it has turned out that this second fac-276 tor is more important, we focus hereafter on HF waves as the target, while the WF cases 277 are detailed in the supplementary document. 278

Name	Notation	Description
Zonal, meridional wind velocity (m.s <sup>-1</sup> ) & temper- ature (K)	$\begin{vmatrix} u_j, v_j & \\ temp_j \end{vmatrix}$	with vertical level $j \in \{0, 2, 9, 19\}$ $(km)$ , where 0 is the surface and 19 is the bal- loon's level.
Total precipitation (m)	tp	at center of horizontal grid points.
Mean & standard devia- tion of precipitation (m)	${{\rm tp}_{{ m mean}}}\ \&\ {{ m tp}_{{ m sd}}}$	over horizontal grid points.
Solar zenith angle (°)	$  sza^1$	at the location of the balloon.
Log surface pressure (log(hPa))	lnsp	at the surface level.

 Table 1.
 Large-scale input data for training ML models.

## 279 **2.4 Evaluation metric**

An important aspect in any comparison of models to observations is the choice of 280 a metric to evaluate the performance of the models. We explain here why, in line with 281 Lott et al. (2023), we use correlation between modelled and observed values as our met-282 ric. The current study is in line with studies that have compared parameterized and ob-283 served gravity waves (eg Geller et al. (2013)). In such comparisons, the first aim is nat-284 urally to compare *mean* momentum fluxes, yet over the past decade the importance of 285 having a realistic variability has been emphasized (Alexander et al., 2010)). This has high-286 lighted the notion of intermittency (Hertzog et al., 2012) and quantification of the dis-287 tribution of momentum fluxes when comparing parameterizations to observations (de la 288 Camara et al., 2014; Bushell et al., 2015). These comparisons, however, concern the over-289 all statistics, not a direct comparison of observed and parameterized variations on a case-290 to-case basis. Obtaining an appropriate observational dataset and gathering the corre-291 sponding large-scale variables for such a case-to-case comparison has required significant 292 work and has been achieved for the comparison of Lott et al. (2023). These datasets pro-293 vide a unique opportunity to investigate the co-variability of observed GWMF and es-294 timations from the large-scale flow, whether based on parameterizations (Lott et al., 2023) 295

<sup>&</sup>lt;sup>1</sup> Solar zenith angle is the only input obtained from the balloons, not from the ERA5. It is a periodic function that provides an estimation of time of the day and the balloon's location.

or on machine learning techniques presented in this study. This is why we here focus on this co-variability, quantified by the correlation. It is expected that the averaging effect of tree-based algorithms may lead to underestimation of the target, especially when dealing with rare extreme values such as GWMFs. Obtaining appropriate intermittency of the reconstructed gravity wave momentum fluxes will require further efforts, and directions for these efforts are discussed in the perspectives (Section 5).

# 302 3 Results

This section reports the correlations of ML methods in reconstructing various types 303 of observed GWMFs. The numerical study is carried out using sklearn.ensemble mod-304 ule in Python (Pedregosa et al., 2011). In general, the three ML models exhibit very com-305 parable performances on any given balloon. In contrast, the performance of the ML mod-306 els varies significantly from one balloon to another. At their best, ML models can achieve 307 an encouraging level of correlation larger than 0.7. The average performance over all bal-308 loons and data exceeds 0.5. The worst performances is found for westward GWMF for 309 a specific balloon, with correlation down to 0.2. Overall, the performances of ML mod-310 els are sensitive to the choice of balloons and the types of GWs being considered (east-311 ward, westward or absolute GWMFs). The numerical results for HF waves are presented 312 in the following subsections, while the WF cases are presented in supplementary doc-313 ument. 314

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# 3.1 Overall performances

Three examples of observed and predicted GWMFs of the HF case are presented 316 in Figure 2 below. Each subplot displays the eastward component of the GWMFs in the 317 positive part and the westward ones in the negative part. It can be observed that the 318 models effectively capture the fluctuations of the observed momentum fluxes, particu-319 larly on balloon 2. However, the models struggle to fully estimate the amplitudes of high-320 peak events, especially for balloons 3 and 7. Overall, the performances of all ML mod-321 els are quite similar; however, there are cases where one outperforms the others. For ex-322 ample, Adaboost appears to do a slightly better job on balloon 2 than the other two mod-323 els in capturing the amplitudes of the high-peak events. It is worth noting that balloon 324 2 presents overall the best performance for the ML models, balloon 7 illustrates a typ-325 ical average case, and balloon 3 is the most challenging one to predict: this is suggested 326 visually in Figure 2, and is confirmed quantitatively in Table 2. 327

A feature of the reconstructed GWMF is that the peak values are generally under-328 estimated, as can be seen even for balloon 2 in Figure 2. This is partly expected given 329 that tree-based models involve averaging from numerous decision trees, some of which 330 are insufficiently informed to capture extreme occurrences of GWMFs. To document the 331 relationship between the reconstructed and observed GWMFs, scatterplots are displayed 332 in Figure 3. These illustrate how the reconstruction captures well the variations of GWMFs, 333 especially for rather weak variations. In contrast, for occurrences of larger MFs, the ob-334 served values cover a range of values that are not captured by the ML approaches. The 335 scatterplots illustrate that those occurrences are rare, and the training data certainly con-336 stitutes a limiting factor. It is not clear that it may be possible to capture, in a deter-337 ministic way, these extremes. It is worth noting that the ML approaches do generally 338 capture when the GWMF is at the high end of the range of reconstructed values. 339

Figure 4 presents boxplots of Pearson's correlation coefficients between predicted and true GWMFs of the HF case. Firstly, choosing the best model is challenging due to the variability in the boxplot positions, which depends on the choices of balloons and GWMF types. For instance, on balloon 2, the correlation boxplot of Adaboost is higher than the other two methods for the absolute and westward cases but lower than Random Forest for the eastward case. However, these differences are generally insignificant



**Figure 2.** Observed and predicted time series of high-frequency east and westward GWMFs of the best, worst and medium cases: balloon 2, 3 and 7, respectively. The x-axis label "Day" indicates the number of days since the individual balloon was launched, with 0 corresponding to the moment of launch.



**Figure 3.** Scatterplots of predictions against observed (true) GWMF corresponding to the time series of Figure 2. Only the predictions of Adaboost are presented for balloon 2, 3 and 7 (from left to right). The lower groups represent the westward fluxes, while the upper groups denote the eastward ones. The red line serves as the reference 1:1 line.

compared to the variations observed between different balloons. Secondly, ML models demonstrate strong performance on balloons 2, 6, and 8 across all types of momentum fluxes, and they also excel in predicting the eastward momentum flux of balloon 1. Nevertheless, balloons 3, 4, 5, and 7 pose greater challenges, with the most difficult being the westward component of GWMF on balloon 3. Finally, the ML models generally outperform the gravity wave drag scheme of the IPSL model (Lott et al., 2023), except for balloon 3 (east and westward) and balloon 4. Moreover, Table 2 provides the statisti-

cal significance of the correlations presented in Figure 4.

	AB	0.43	0.70	0.18	0.37	0.50	0.57	0.32	0.64
Vestward	ET	0.37	0.63	0.23	0.33	0.40	0.72	0.45	0.66
Δ	$\mathrm{RF}$	0.38	0.60	0.21	0.35	0.35	0.68	0.44	0.66
	AB	0.67	0.65	0.43	0.44	0.35	0.70	0.42	0.68
Eastward	ET	0.69	0.62	0.49	0.48	0.48	0.65	0.49	0.71
	RF	0.67	0.67	0.41	0.47	0.39	0.64	0.46	0.71
0	AB	0.58	0.74	0.49	0.47	0.55	0.75	0.48	0.72
Absolute	ET	0.57	0.67	0.48	0.43	0.56	0.74	0.53	0.76
	RF	0.56	0.70	0.45	0.44	0.51	0.72	0.51	0.74
Duration/	DOF	107/53	103/51	101/33	67/22	79/19	57/10	83/16	77/12
Бъд	niid	28/02/20	23/02/20	28/02/20	02/02/20	23/02/20	01/02/20	28/02/20	22/02/20
Ctort	Juarc	12/11/19	11/11/19	18/11/19	27/11/19	05/12/19	06/12/19	06/12/19	07/12/19
4 I+	AIN	20.7	20.2	19.0	18.8	18.9	20.5	20.2	20.2
Flicht	r ugut	01_STR1	02_STR2	$03_{-}TTL3$	04_TTL1	$05_{-}TTL2$	$06\_STR1$	$07\_STR2$	$08\_STR2$





**Figure 4.** The boxplots display the correlations between predicted and observed high-frequency GWMFs obtained from 50 runs of ML methods as shown in Table 2. For each balloon, moving from left to right, the three boxplots correspond to the Random Forest, Extra Trees, and AdaBoost methods, respectively. The dashed horizontal red lines indicate the performance of the parameterization of the IPSL model (Lott et al., 2023).

## 3.2 Which large-scale inputs are informative for ML models?

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The tree-based ensemble ML models employed in this study are not only proficient in predicting GWMFs but also offer valuable insights into the importance of large-scale input information during their training process. Each method exploits the feature importance (decrement of impurity measure at each split) of its individual decision trees for determining the overall feature importance, resulting in a ranking of input features from most to least important. Figure 5 showcases the ranking of the top 5 input features for all ML methods and GWMF types of the HF case.

Generally, the high-ranking inputs consist of variables that describe precipitation 362 and wind velocity at and below the balloon's level. It is important to note that differ-363 ent models may not rank input features in the same way for a given target (as seen along 364 the rows), due to the variations in the way individual trees are grown. However, the three 365 models concur on the strongly impactful input features; for example, wind velocity at 366 the balloon's level (u19) ranked first in the eastward case (second row) for all models. 367 This suggests that the wind velocity surrounding the balloons is the most informative 368 large-scale variable for predicting eastward gravity wave momentum fluxes (GWMFs). 369 Furthermore, the few most significant inputs show a similar preference in both absolute 370 and eastward GWMFs within the same model, as demonstrated in the columns of the 371 first and second rows. For instance, standard deviation and average total precipitation 372



**Figure 5.** The boxplots show the 5 most important features given by different ML models (by column) on different types of targets (by row). Each boxplot is obtained from the same 50 simulations as displayed in Figure 4.

(tp\_sd and tp\_mean) are identified as impactful inputs in random forests, while surface zonal wind velocity (u0) is deemed the most important one in extra trees.

#### 375 4 Discussion

While the results of the machine-learning models are generally encouraging, deficiencies and cases with poor performances were also found. The main motivation for this study being to probe the relationship between the large-scale and the unresolved process, these somewhat negative results are also of interest and can provide useful insights. Possible explanations for the main difficulties encountered are discussed below.

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## 4.1 Why are westward GWMFs more challenging?

Figure 4 displays the performances of the ML models and those of the parameter-382 ization used in the IPSL climate model. Balloon 4 constitutes an exception, for which 383 the parameterization systematically performs better than the ML methods. Leaving bal-384 loon 4 aside, ML approaches unambiguously outperform the parameterization for the ab-385 solute momentum fluxes. For the eastward momentum fluxes, ML approaches generally 386 perform better or are similar to the parameterization. In contrast, both ML approaches 387 and the parameterization have poorer performances for westward MF, and with greater 388 variability for both: for five balloons, ML outperforms clearly the parameterization, whereas 389 for two balloons (including balloon 4) the parameterization clearly outperforms the ML. 390 The present section discusses possible reasons for this difficulty in reproducing the west-391 ward momentum fluxes. 392

Figure 6 displays the Probability Density Function of winds for three balloons as 393 blue curves: balloon 2 has flown in winds that include a majority of westward, strong 394 winds. Like balloon 1, it traveled near 10°S in easterly flow for a significant portion of 395 its flight. In contrast, balloons 3 and 7 have flown in weaker winds, with a mild dom-396 inance of westerly winds. Also plotted in Figure 6 are conditional PDFs of the zonal winds, 397 conditioned on the intensity of the absolute GWMF. The purpose is to detect if strong 398 values of GWMF were associated to specific wind conditions. For balloon 2, strong GWMF 399 values were found mostly for moderate to strong easterly winds, and this distribution 400 is insensitive to the quantile chosen for the GWMF (90th, 95th or 99th percentile). For 401 balloon 7, the distribution is somewhat sensitive to the quantile chosen. Finally, for bal-402 loon 3, the conditional distribution of zonal wind dramatically changes when it is restricted 403 to the 99th percentile. This detects a particularly intermittent time series, with variabil-404 ity dominated by one extreme event, as seen from Figure 2. These findings contribute 405 to explaining the poor performances for balloon 3: the variability of GWMF was dom-406 inated there by one (or very few) extreme events, occurring in a specific condition with 407 very weak winds (close to zero, less than 5 m. $s^{-1}$ ). In contrast, the good performances 408 for balloon 2 occur in a case with less intermittency, for which large GWMF are found 409 in strong (easterly) winds. 410



Figure 6. Conditional densities of zonal wind given different values of high-frequency westward GWMFs. Here, q(0.9), q(0.95) and q(0.99) are the 90%, 95% and 99% quantiles of the absolute value of high-frequency westward GWMFs, respectively.

From Table 2, Figure 4 and the trajectories of the balloons (Corcos et al., 2021), it appears that drifting with easterly winds may constitute a favorable factor (balloon 2), but neither a sufficient one (the correlation for westward momentum fluxes for balloon 1, which has a similar trajectory, is moderate, 0.43 at most) nor a necessary one: balloons 6 and 8 generally drift eastward, but good performances are found for the ML reconstruction of the westward MF (0.66 and 0.72 respectively).

Another aspect that influences the performances is the geographical location, and 417 more specifically the latitude of the balloons. Figure 7 displays the PDF of latitude for 418 the eight balloons, distinguishing those for which the ML reconstruction of westward MF 419 is satisfactory (balloons 1, 2, 6 and 8, full lines) from those for which it remains chal-420 lenging (balloons 3, 4, 5 and 7). Here again, one does not isolate a necessary condition, 421 but the balloons for which reconstruction remain challenging are those that remain clos-422 est to the equator. This is consistent with the general expectation that dynamics is more 423 complicated near the Equator, although it is not completely clear why this should mat-424 ter for a small-scale process such as convectively generated gravity waves. It may be that 425 it is not the dynamics itself that is intrinsically more difficult to capture at the Equa-426 tor: it may be the input variables that are poorer, less accurate, very close to the Equa-427 tor. It is known indeed that significant errors, in particular in the wind, are present in 428 the reanalyses very near the Equator (Podglajen et al., 2014; Baker et al., 2014; Ern et 429 al., 2023) and the errors are enhanced within a few degrees of the Equator (roughly be-430 tween  $8^{\circ}S$  and  $8^{\circ}N$ ). 431

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## 4.2 Why are some balloons easier to predict than others?

Figure 7 indicates that the predictability of the observed GWMFs is influenced by
the balloons' position, specifically, their distances from the equator. Balloons that traveled farther from the equator, primarily south (except for balloon 6, which also explored
farther to the north), were found to be easier to predict. This tendency is observed for
balloons 1, 2, 6, and 8 which are the well-predicted balloons. In contrast, the challenging balloons spent most of their time flying within a few degrees of the equator, where
the atmospheric conditions are not well described by ERA5 data.



**Figure 7.** The trajectories of the balloons during the whole flight (a), and their latitude PDFs (b) and (c). Dashed lines correspond to balloons that pose challenges in prediction.

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## 4.3 Exploring potential reasons for unsatisfactory cases

Several factors are expected to limit the ability to estimate the observed GWMFs from inputs describing the large-scale flow:

- A. Part of the relationship between the large-scale flow and a subgrid-scale process such as gravity waves is non-deterministic, or stochastic: for given values of the large-scale fields, a range of different realizations of the subgrid-scale process is possible. It depends on the process: orographic gravity waves are likely more predictable than convective processes for instance.
- B1. The estimate of GWMFs from superpressure balloons is very local and samples
  only along its trajectory. This is only partly mitigated by the hourly averaging.
  The GWMFs time series certainly remain sensitive to the specific location of the
  balloon. At present, it is difficult to estimate this sensitivity. Investigations with
  virtual balloons in high-resolution simulations shall be informative on this issue.
- B2. A second concern regarding the target used for the ML is the observational error
  present in the estimates of the GWMFs from balloon measurements. These estimates are regarded as accurate because several variables are measured simultaneously and because of the quasi-Lagrangian nature of the measurements (Geller
  et al., 2013; Vincent & Hertzog, 2014). There remains nonetheless observational
  error.
- C1. Concerns are also present for the input variables, and in particular it is known that
   the description of the equatorial dynamics is challenging, with significant errors
   remaining present in the reanalysis especially for wind (Podglajen et al., 2014).
  - C2. Another concern regarding input variables is that we may have omitted variables that could have been informative.

In our study, we mitigated the concern of omitting informative variables (C2.) by initially training ML models on a large set of ERA5 inputs, then selectively reducing them to a reasonably small subset, as described in Section 2.1. This approach ensures that essential ERA5 inputs are not inadvertently omitted. Furthermore, fine-tuning the hyperparameters of the models enhances their predictive capacity. Regarding the concern of large-scale variables (C1.), a sensitivity test to the error of ERA5's wind is described at the end of Section 5 (key messages).

In addition, we observe that all the balloons often flew over many convective pro-471 cesses, and the high-peak events often correspond to deep convective systems, as illus-472 trated for selected cases in Figure 8 below. On January 12th, 2020, balloon 2 was fly-473 ing in an area of convection (upper panels (a1) and (a2)), which is likely responsible for 474 the highest peaks in its GWMF time series. Interestingly, for balloon 2, almost all events 475 correspond very well with precipitation as described by ERA5 (first column of Figure 9). 476 On the contrary, there is only one big event that happened for balloon 3 around Jan-477 uary 29th, 2020 (lower left panel (b)). However, the ML models failed to capture it, as 478 it appears to be absent from the ERA5 input variables (not reflected in precipitation nor 479 winds as shown in the second column of Figure 9). This is also true for other challeng-480 ing balloons, such as the 4th and 5th. Regarding balloon 7, the large-scale flow provide 481 partial information for the high-peak events, resulting in partial success in the model's 482 predictions. 483

## <sup>484</sup> 5 Conclusion and perspectives

## 5.1 Key messages

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The relationship between the large-scale atmospheric flow and gravity waves in the lower stratosphere has been investigated using Machine Learning (ML) approaches. This relationship is accounted for in global models through *parameterizations*. ML approaches allow us to revisit these in several ways, notably investigating how much of the subgridscale signal may be estimated *deterministically*, and which are the key variables for that purpose.



Figure 8. Brightness temperature from NOAA/NCEP GPM\_MERGIR product (Janowiak, 2017), positions, and the corresponding observed GWMFs at the high-peak events of balloon 2 (top), balloon 3 (lower left) and balloon 7 (lower right).



Figure 9. Time series of absolute GWMFs and the most informative ERA5 inputs in daily time resolution. The clear correspondence between precipitation and GWMF of balloon 2 can be visually observed in column (a). In contrast, this is not the case at all for balloon 3 as shown in column (b), and it partially presents in column (c) of balloon 7.

492 493 Estimates from superpressure balloon measurements were chosen as the target observations for gravity wave momentum fluxes (GWMF). The first campaign of the Strateole 2 project (Haase et al., 2018) consisted of eight balloons flying an average of about
85 days each around the globe in the equatorial band. The quasi-Lagrangian nature of
the balloons allows an accurate estimate of gravity wave momentum fluxes (Geller et al.,
2013), the latter being a key quantity for parameterizations (Alexander et al., 2010). Analysis of the GWMF estimated from measurements in this first campaign has highlighted
and confirmed convection as the main source of gravity waves in this region, especially
for waves with high frequencies (periods shorter than one hour); see Corcos et al. (2021).

The description of the large-scale flow environment was provided from the ERA5 reanalysis, along with vertical profiles co-located with each balloon at each time. These variables included wind, pressure, temperature, and precipitation. The latter being a noisy and uncertain field, values of total precipitation were retrieved in a 500 × 500 km<sup>2</sup> area around each balloon location, and was generally described by the mean and standard deviation over this area.

The ML models used are tree-based methods: random forests, extremely randomized trees, and adaptive boosting. Other methods were also investigated, as sensitivity experiments, without yielding major improvements. For each method, seven out of eight balloons were used for *training*, and the last balloon was used for *testing*.

The main results obtained from these investigations are as follows:

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- 1. Based on the information provided by the large-scale flow data from ERA5, ML 512 methods can reconstruct the observed GWMFs with correlations exceeding 0.7 in 513 certain cases (balloon 2, 6, and 8), which is encouraging. Overall, the majority of 514 the correlations are statistically significant at least at the 95% level, except for a 515 few cases, as indicated in Table 2. The performances of ML methods, however, 516 vary considerably from one balloon to another, with correlations down to 0.4 for 517 some other balloons, and even down to 0.2 in one case. The overall average cor-518 relation for the HF case is 0.54, while a slightly lower average correlation of 0.49519 is obtained in the WF case. In general, the correlations for WF waves are slightly 520 weaker than those for HF waves (refer to the supplementary document for details). 521
- 2. The variations in performance are much larger between different balloons, than they are for a given balloon between ML approaches. This suggests that the performances are limited by the datasets, not by the choice of ML approach. The treebased methods proved generally efficient, but there is not an overwhelming preference for one of them. Adaptive boosting frequently performed a bit better, but all three failed to capture the intensity of the (very intermittent) peaks in GWMF.
- 3. The most informative explanatory variables are those describing the precipitation 528 and the zonal wind at and below the balloon's level. It is indeed an advantage of 529 tree-based methods to provide information about the usefulness of the different 530 inputs, e.g. through the Gini importance (Hastie et al., 2001). The importance 531 of precipitation is consistent with the convective generation of the waves (Lott & 532 Guez, 2013; Corcos et al., 2021). The importance of winds is consistent with the 533 general understanding of the generation and propagation of waves (Kim et al., 2003); 534 the relevance of wind at the balloon level is reminiscent of previous findings (Plougonven 535 et al., 2017; Amiramjadi et al., 2023). 536
- 4. The ML methods were more efficient at reconstructing the part of GWMF associated with high-frequency waves (periods shorter than an hour) than the whole
   spectrum. This is consistent with the local character of the explanatory variables
   provided as inputs: high-frequency waves will be shorter-lived and propagate more
   vertically.
- 5. Different decompositions of the GWMF were used: absolute, eastward and west-ward GWMF. Interestingly, the performances significantly differed between these.
  The most difficult to reconstruct was found to be westward GWMF. Reasons for this likely include limitations of the dataset, to be further discussed below.

However, there are still parts where the large-scale flow are not informative enough
in the estimation. There are cases where high peaks are present in the observed target,
which indicates interesting events; however, large-scale flow are missed to describe them.
As a result, the models failed to reconstruct such events in GWMFs (balloon 1 and 3,
for example).

In addition, we have also implemented ML models by replacing ERA5's winds with 551 balloon-observed winds at the balloon's level. This tests the sensitivity to errors in the 552 input variables, for the variables for which we have direct observations, and which is known 553 in the reanalysis to include significant error. The results suggest there is some sensitiv-554 ity, but it is not extensive. Overall, the performances on some challenging balloons such 555 as balloon 3 and 5 are significantly improved when using observed winds instead of ERA5's 556 winds. In contrast, the performance on balloon 8 drops quite a bit compared to the model 557 with ERA5's winds. Overall, the models utilizing observed wind achieve an average cor-558 relation of 0.53 in the HF case and 0.47 in the WF case. These results can be found in 559 the supplementary document. 560

## 5.2 Perspectives

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Although the ML approaches have performed well, and nearly always better than 562 the parameterization, there are clear limitations to the current investigation, calling for 563 further research. The very strong sensitivity of the performances to the balloon that is 564 left out and then used for testing is a clear indication that we lack data: the results strongly 565 depend on the split of the data for training and testing, the performances are far from 566 convergence. This is consistent with the strong intermittency of the GWMF (Hertzog et al., 2012; Plougonven et al., 2013) and with the illustrative time series of Figure 2: 568 for each balloon, GWMF are dominated by a few events, such that even with 680 days 569 of balloon measurements, only a few handfuls of GWMF peaks are described. This is 570 too little for data-driven methods. This also explains why clear distinctions between the 571 different methods are not found: the ML methods do their best but still lack data to clearly 572 separate a better method for this problem, if there is one. 573

574 Ways forward include:

Obtaining more observations to use as the target, keeping the same framework for the ML. Additional observations would come from the second Strateole 2 campaign (in 2021) and from Loon balloons (Schoeberl et al., 2017; Köhler et al., 2023). The additional Strateole data would enhance the data by less than a factor 2 and is therefore not expected to suffice to make a dramatic change. The Loon data would come with other difficulties as the observations were not made for research purposes and come with their own challenges (Green et al., 2023).

Additional data could be provided not for the targets, but for the explanatory vari-582 ables. A first step could be including additional input variables from the reanal-583 yses. However, preliminary attempts have not suggested significant gains from the 584 most evident additional culprits. A second step would consist of providing much 585 more detailed and more accurate information about the background flow: this could 586 be obtained from satellite observations, such as the observations of brightness tem-587 peratures from geostationary satellites shown in Figure 8. This would constitute 588 a very interesting new study but in a profoundly new framework and with differ-589 ent aims: to fully use the information available from satellites would a priori re-590 quire providing maps (or images, or 2D fields) as input variables (more akin to 591 Matsuoka et al. (2020), although their inputs were from models, not observations). 592 The ML used would need to be reassessed (Matsuoka et al. (2020) used neural net-593 works, for instance). Such a study would be of great interest because the perfor-594 mance of the ML methods would much less be tainted by the uncertainty (or er-595 rors) present in the inputs that serve to describe the background. Additionally, 596

much more detailed information would be provided about the background flow, allowing the ML methods to tap into a greater reservoir of potentially relevant information, and hence providing more precise answers regarding the relationship of the large-scale flow to the gravity wave signal. However, if the outcome of such an exercise would be of interest fundamentally, it would be more removed from the framework in which current parameterizations operate.

- A shortcoming of the present ML approaches is that they underestimate the peak 603 values for GWMF (see Figures 2 and 3. This is expected, given the averaging in-604 volved in tree-based method and the limited number of strong events present in 605 the training data. However, this implies that the distribution of reconstructed momentum fluxes misses the tail of intense, rare events, which are known to matter 607 for atmospheric gravity waves (Hertzog et al., 2012; de la Camara et al., 2016). 608 One way to overcome this would be to aim not at a deterministic reconstruction 609 of the momentum fluxes, but at reconstructing a probability density function of 610 these. This change of framework, equivalent to changing from a deterministic to 611 a stochastic parameterization, would in fact be more consistent for three reasons: 612 first, given some large-scale conditions, there are certainly several different small-613 scale configurations with different resulting gravity waves that can occur. Second, 614 for any given realization of the small-scale flow corresponding to large-scale con-615 ditions, our observed values depend on the specific sampling by the balloon. At 616 present, we do not fully know how sensitive the observed gravity wave momen-617 tum fluxes are to this sampling. Finally, the estimate of gravity wave momentum 618 fluxes from the observed balloon measurements involves assumptions and method-619 ological choices, and there is as always an observational error in the estimates for 620 GWMF. Given that the ML methods do capture rather well the occurrence of larger 621 values, using ML methods to reconstruct a PDF of likely fluxes, rather than a sin-622 gle, deterministic value, could give room to better represent the observed GWMF, 623 although only in a probabilistic way. 624
- A fourth way forward consists in applying similar investigations on datasets where 625 more data is available, albeit at the cost of more uncertainty on the realism of the 626 data. High-resolution models such as global convection permitting simulations (Stephan 627 et al., 2019) provide a wealth of information on the resolved gravity wave field, 628 and many studies have repeatedly highlighted the ability of models to simulate 629 efficiently many features of the observed gravity wave field (Plougonven & Teit-630 elbaum, 2003; Wu & Eckermann, 2008; Preusse et al., 2014; Stephan et al., 2019). 631 Model output from global simulations would provide amounts of data for which 632 the sampling limitations of the Strateole balloons would not be present. The down-633 side is the limitations of model data, relative to observations, and the need for strate-634 gies to validate which aspects of the simulations are realistic. 635

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## 643 6 Open research

Balloon data used in this study are presented in Haase et al. (2018) of the STRA-TEOLE 2 mission and can be extracted from the following website: https://webstr2 .ipsl.polytechnique.fr. The ERA5 input variables are described in Hersbach et al. (2020) and can be obtained from the COPERNICUS access hub using the following website: https://scihub.copernicus.eu/. The machine learning algorithms implemented
in our analysis are available in the scikit-learn Python library (Pedregosa et al., 2011)
and can be downloaded from its website: https://scikit-learn.org/stable/install
.html. Finally, the source codes for implementing machine learning methods in our analysis are made available at the following GitHub repository: https://github.com/hassothea/

Reconstruction\\_of\\_GWMF\\_using\\_ML\\_ERA5.

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