

Journal of Statistical Software

MMMMMM YYYY, Volume VV, Issue II.

doi: 10.18637/jss.v000.i00

modelimportance: An R package for evaluating model importance within an ensemble

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Abstract

Ensemble forecasts are commonly used to support decision-making and policy planning across various fields because they often offer improved accuracy and stability compared to individual models. As each model has its own unique characteristics, understanding and measuring the value each constituent model adds to the overall accuracy of the ensemble is of great interest to building effective ensembles. The R package **modelimportance** provides tools to quantify how each component model contributes to the accuracy of ensemble performance for different forecast types. It supports multiple functionalities; it allows users to specify which ensemble approach to implement and which model importance metric to use. Additionally, the software offers customizable options for handling missing values. These features enable the package to serve as a versatile tool for researchers and practitioners aiming to construct an effective ensemble model across a wide range of forecasting tasks.

Keywords: ensemble, forecast, prediction, model importance, Shapley value, R.

1. Introduction

Ensemble forecasting is a method to produce a single, consolidated prediction by combining forecasts generated from different models. This technique it utilizes each model's strengths to counterbalance their individual weaknesses, leading to more robust and accurate predictions (Gneiting and Raftery 2005; Hastie et al. 2001; Lutz et al. 2019; Viboud et al. 2018). Specifically, ensembles aggregate diverse insights from various models and effectively handle individual models models biases and variances by averaging them out, which can reduce pre-

diction errors and improve overall model performance. These enhanced prediction accuracy and robustness enable ensemble forecasting to be widely used across various domains such as weather forecasting (Jordan A. Guerra et al. 2020; Gneiting and Raftery 2005), financial modeling (Sun et al. 2020; He et al. 2023), and infectious disease outbreak forecasting (Ray and Reich 2018; Reich et al. 2019) to improve decision-making and achieve more reliable predictions. For example, throughout the COVID-19 pandemic, the US COVID-19 Forecast Hub collected individual models developed by over 90 different research groups and built a probabilistic ensemble forecasting model for COVID-19 cases, hospitalizations, and deaths in the US based on those models' predictions, which served as the official short-term forecasts for the US Centers for Disease Control and Prevention (CDC) (Kim et al. 2024).

The quality of forecasts is assessed by evaluating their error, bias, sharpness, and/or calibration using different scoring metrics. The selection of the scoring metrics depends on the type of forecast, such as point forecasts and probabilistic forecasts, and their corresponding formats, such as median/mean, quantiles, and predictive cumulative distribution functions. In the case of point forecasts, accuracy is commonly measured by the mean absolute error (MAE) and the mean squared error (MSE), which are direct assessment tools that calculate the average magnitude of forecast errors. Probabilistic forecasts are typically assessed using proper scoring rules, which consider the uncertainty and variability in predictions, providing concise evaluations through numerical scores (Gneiting and Raftery 2007). Some examples include the weighted interval score (WIS) for the quantile-based forecasts and the continuous ranked probability score (CRPS) for the forecasts taking the form of predictive cumulative distribution functions (Bracher et al. 2021).

Several R packages have been developed for this purpose. To name a few, the forecast package (Hyndman and Khandakar 2008) is widely used for univariate time series forecasting and includes functions for accuracy measurement. The Metrics (Hamner and Frasco 2018) and MLmetrics (Yan 2024) provide a wide range of performance metrics specifically designed for evaluating machine learning models. The scoringRules (Jordan et al. 2019) package offers a comprehensive set of proper scoring rules for evaluating probabilistic forecasts and supports both univariate and multivariate settings. The scoringutils (Bosse et al. 2022) package offers additional features to the functionality provided by scoringRules, which makes it more useful for certain tasks, such as summarizing, comparing, and visualizing forecast performance. Additionally, the scoringutils supports forecasts represented by predictive samples or quantiles of predictive distributions, allowing for the assessment of any forecast type, even when a closed-form expression for a parametric distribution is not available. These packages have been valuable to evaluate individual models as independent entities, using performance metrics selected for each specific situation or problem type. However, they do not measure the individual models' contributions to the enhanced predictive accuracy when used as part of an ensemble. Kim et al. (Kim et al. 2024) demonstrate that a model's individual performance does not necessarily correspond to its contribution as a component within an ensemble. Our developed package introduces this capability. The modelimportance package provides tools to evaluate the role of each model as an ensemble member within an ensemble model, rather than focusing on the individual predictive performance per se.

In ensemble forecasting, certain models contribute more significantly to the overall predictions than others. Assessing the impact of each component model on ensemble predictions is methodologically similar to determining variable importance in traditional regression and

machine learning models, where variable importance measures evaluate how much individual variables enhance the model's predictive performance. R packages that implement these functions include randomForest (Liaw and Wiener 2002), caret (Kuhn 2008), xgboost (Chen et al. 2024), and gbm (Ridgeway and Developers 2024), each providing variable importance measures for different types of models: random forest models, general machine learning models, extreme gradient boosting models, and generalized boosted regression models, respectively. Similarly, the tools in the modelimportance package quantify the contribution of each component model within an ensemble to the ensemble model's predictive performance. They assign numerical scores to each model based on a selected metric that measures forecast accuracy, depending on the forecast type.

These capabilities provide unique support for hub organizers, such as the CDC in the US and the European Centre for Disease Prevention and Control in the EU. These organizations can create more effective ensemble forecasts by gathering and utilizing forecasts from various models based on the precise evaluation of each model's contribution via the **modelimportance** package. This, in turn, facilitates better communication with the public and decision-makers and enhances the overall decision-making process. Specifically, **modelimportance** is incorporated into the 'hubverse', which is a collection of open-source software and data tools developed to promote collaborative modeling hub efforts and reduce the effort required to set up and operate them (Consortium of Infectious Disease Modeling Hubs 2024). This package adheres to the model output formats specified by the hubverse convention, which enables seamless integration and interoperability with other forecasting tools and systems.

The paper proceeds as follows. In Section 2, we address the model output formats proposed within the hubverse framework and the structure of forecasts, followed by a motivating example. Section 3 presents two algorithms implemented in **modelimportance** for calculating the model importance metric: leave-one-model-out and leave-all-subsets-of-models-out. We demonstrate the various functionalities **modelimportance** supports in Section 4 and give some examples in Section 5. We close this paper with some concluding remarks and a discussion of possible extensions.

2. Data

2.1. Model output format

Model outputs are structured in a tabular format designed specifically for predictions. In the hubverse standard, each row represents an individual prediction for a single task, and its details are described in multiple columns through which one can identify the model IDs, task characteristics, prediction representation type, and predicted values (Shandross et al. 2024). In Table 1, for example, the model_id column contains the uniquely identified name of the model that produced the prediction in each row. Task characteristics are represented by reference_date, target, horizon, location, and target_end_date columns, collectively referred to as the task ID columns. The prediction representation type is specified in the output_type and output_type_id columns. This example illustrates short-term forecasts of incident influenza hospitalizations in the US for Massachusetts (FIPS code 25), generated by the model 'Flusight-baseline' on November 19, 2022. The forecasts are provided in seven

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model_id	reference_date	target	horizon	location	target_end_date	output_type	output_type_id	value
Flusight-baseline	2022-11-19	wk inc flu hosp	0	25	2022-11-19	quantile	0.05	22
Flusight-baseline	2022-11-19	wk inc flu hosp	0	25	2022-11-19	quantile	0.1	31
Flusight-baseline	2022-11-19	wk inc flu hosp	0	25	2022-11-19	quantile	0.25	45
Flusight-baseline	2022-11-19	wk inc flu hosp	0	25	2022-11-19	quantile	0.5	51
Flusight-baseline	2022-11-19	wk inc flu hosp	0	25	2022-11-19	quantile	0.75	57
Flusight-baseline	2022-11-19	wk inc flu hosp	0	25	2022-11-19	quantile	0.9	71
Flusight-baseline	2022-11-19	wk inc flu hosp	0	25	2022-11-19	quantile	0.95	80
Flusight-baseline	2022-11-19	wk inc flu hosp	1	25	2022-11-26	quantile	0.05	5
Flusight-baseline	2022-11-19	wk inc flu hosp	1	25	2022-11-26	quantile	0.1	21
Flusight-baseline	2022-11-19	wk inc flu hosp	1	25	2022-11-26	quantile	0.25	38

Table 1: Example of the model output for incident influenza hospitalizations extracted from forecast_outputs data in the hubExamples package.

Output Type	Scoring Rule	Description
mean median quantile pmf	MSE MAE WIS Log Score	Evaluate using the mean squared error (MSE) Evaluate using the mean absolute error (MAE) Evaluate using the weighted interval score (WIS) Evaluate using the logarithm of the probability assigned to the true outcome (LogScore)

Table 2: Pairs of output types and their associated scoring rules for evaluating prediction performance.

quantiles (0.05, 0.1, 0.25, 0.5, 0.75, 0.9, 0.95) for each target end date.

2.2. Structure of forecasts

The forecasting model supports multiple output types. Generally, quantitative forecasts can be categorized into either point forecasts or probabilistic forecasts. For a specific task, point forecasts, represented by a single predicted value, provide a clear and concise prediction, making them easy to interpret and communicate. Probabilistic forecasts, on the other hand, describe the likelihood of different outcomes, conveying the uncertainty inherent in the prediction. These forecasts are represented by a probability distribution over possible future values in various ways, such as probability mass functions (pmf), cumulative distribution functions (cdf), or probability quantiles (or intervals).

The output_type and output_type_id columns in the model output format, as defined by the hubverse convention, specify the forecast structure. The output_type column takes the character value 'mean' or 'median' for point forecasts, and 'pmf', 'cdf', or 'quantile' for probabilistic forecasts. The output_type_id column provides additional details for probabilistic forecasts; for instance, when the output_type is 'quantile', the output_type_id identifies specific quantile levels, as illustrated in Table 1. In the case of point forecasts, output_type_id column has 'NA'. Different output types correspond to different scoring rules for evaluating a model's prediction performance. Table 2 presents the output types and their associated scoring rules supported by the **modelimportance** package.

3. Algorithms

This section provides a brief description of the leave one model out (LOMO) and leave all subsets of models out (LASOMO) algorithms. (Details can be found in Kim *et al.* (2024))

LOMO involves creating an ensemble by excluding one component model from the entire set of models. Let A be a set of n models and F^i be a forecast produced by model i, where $i=1,2,\ldots,n$. Each ensemble excludes exactly one model while including all the others. Denoting by $F^{A^{-i}}$ an ensemble forecast constructed without F^i and by F^A the ensemble forecast built from the entire set of models, the importance score using LOMO is calculated by the difference of measures of these two ensemble performances, $F^{A^{-i}}$ and F^A . For example, when evaluating model 1 within an ensemble of three models (n=3), LOMO creates an ensemble forecast $F^{\{2,3\}}$ using only F^2 and F^3 . The performance of this reduced ensemble is then compared to the full ensemble forecast $F^{\{1,2,3\}}$, which incorporates all three models.

On the other hand, LASOMO involves ensemble constructions from all possible subsets of models. For each subset S that does not contain the model i, $S \cup \{i\}$ plays a role of A in the LOMO; the score associated with the subset S is the difference of measures between F^S and $F^{S \cup \{i\}}$. Then, all scores are aggregated across all possible subsets that the model i does not belong to. For example, using the earlier setup of three forecast models, LASOMO considers three subsets, $\{2\}$, $\{3\}$, and $\{2,3\}$, to calculate the importance score of model 1 (excluding all subsets that include model 1). The ensemble forecasts $F^{\{2\}}$, $F^{\{3\}}$, and $F^{\{2,3\}}$ are then compared to $F^{\{1,2\}}$, $F^{\{1,3\}}$, and $F^{\{1,2,3\}}$, respectively. The performance differences attributable to model 1's inclusion are aggregated, which results in the importance score of model 1. We note that the subsets may have different weights during the aggregating process. The **modelimportance** package offers two weighting options for subsets: one assigns equal (uniform) weights to all subsets, and the other assigns weights based on their size, similar to the concept of Shapley values. Users can choose one to evaluate the contribution of each model in a manner suited to their preferred framework.

Algorithm 1 Importance score using leave one model out (LOMO) algorithm

Input:

- Set of n individual models, $A = \{1, 2, ..., n\}$, and their forecasts $\{F^1, F^2, ..., F^n\}$
- Truth value, y
- \bullet Function q to build an ensemble
- Scoring rule ψ to evaluate forecast skills

Output: importance metric of model i, $\phi^{i,\text{lomo}}$

- 1: Create an ensemble forecast F^A using $g: F^A \leftarrow g(\{F^1, F^2, ..., F^n\})$
- 2: Evaluate F^A using ψ : $\psi(F^A, y)$.
- 3: **for** each i, (i = 1, 2, ..., n) **do**
- 4: $F^{A^{-i}} \leftarrow g(\{F^j | j \neq i, j \in A\})$
- 5: Compute $\psi(F^{A^{-i}}, y)$.
- 6: $\phi^{i,\text{lomo}} \leftarrow \psi(F^{A^{-i}}, y) \psi(F^A, y)$
- 7: end for

Algorithms 1 and 2 outline the steps to implement LOMO and LASOMO for a single prediction task, respectively.

Algorithm 2 Importance score using leave all subsets of models out (LASOMO) algorithm
Input:

- Set of n individual models, $A = \{1, 2, ..., n\}$, and their forecasts $\{F^1, F^2, ..., F^n\}$
- Truth value, y
- \bullet Function g to build an ensemble
- Scoring rule ψ to evaluate forecast skills

Output: Importance metric of model $i, \phi^{i,\text{lasomo}}$

```
1: for i = 1 to n do
           \phi^{i,\text{lasomo}} \leftarrow 0
 2:
           Make a list of non-empty subsets of A that does not contain i: S_1, S_2, \dots, S_{2^{n-1}-1}
 3:
           for j = 1 to 2^{n-1} - 1 do
  4:
               Assign a weight to the subset S_j:
  5:
                \begin{array}{c} \textbf{if} \ \textbf{all} \ \textbf{subsets} \ \textbf{have} \ \textbf{uniform} \ \textbf{weights} \ \textbf{then} \\ 1 \end{array} 
  6:
               \begin{array}{l} \gamma_{S_j} \leftarrow \frac{1}{2^{n-1}-1} \\ \textbf{else} \ (\textit{subset's weight depends on its size}) \end{array}
  7:
 8:
                  \gamma_{S_j} \leftarrow \frac{1}{(n-1)\binom{n-1}{|S_j|}}
 9:
               end if
10:
               F^{S_j} \leftarrow g(\{F^j|j \in S_i\})
11:
               F^{S_j \cup \{i\}} \leftarrow g(\{F^i, F^j | j \in S_i\})
12:
               Compute \psi(F^{S_j}, y) and \psi(F^{S_j \cup \{i\}}, y)
13:
               \phi^{i, \text{lasomo}} \leftarrow \phi^{i, \text{lasomo}} + \gamma_{S_i} \times \left[ \psi(F^{S_j}, y) - \psi(F^{S_j \cup \{i\}}, y) \right]
14:
           end for
15:
16: end for
```

4. Main funtion: Evaluating ensemble members

In this section, we describe the functionalities of the main function model_importance(), where multiple options are available to customize the evaluation framework (Table 3).

forecast_data is a data frame containing predictions and should be or can be coerced to a model_out_tbl format, which is the standard S3 class model output format defined by the hubverse convention. Only one output_type is allowed in the data frame, and it must be one of the mean, median, quantile, or pmf.

oracle_output_data is a data frame containing the ground truth data for the variables that

Argument	Description	Possible Values	Default
forecast_data	Forecasts	Must be the model output format	N/A
oracle_output_data	Ground truth data	Must be the oracle output format	N/A
ensemble_fun	Ensemble method	simple_ensemble, linear_pool	simple_ensemble
training_window_length	Time interval of historical data used during the training process	Non-negative integer	0
<pre>importance_algorithm</pre>	Algorithm to calculate importance	lomo, lasomo	lomo
subset_wt	Method for assigning weight to subsets when using lasomo algorithm	equal, perm_based	equal
na_action	Method to handle missing data	worst, average, drop	worst
•••	Optional arguments for simple_ensemble	Varies	agg_fun = mean

Table 3: Description of the arguments for the model_importance() function, including their purpose, possible values, and default settings.

are used to define modeling targets. This data must follow the oracle output format, which includes independent task ID columns (e.g., location, target_date, and age_group), the output_type column specifying the output type of the predictions and an oracle_value column for the observed values. If the output_type is either "quantile" or "pmf", the output_type_id column is required to provide further identifying information. For "quantile", it should contain numeric values between 0 and 1 indicating quantile levels (e.g., "0.1", "0.25", "0.5", "0.75", "0.9"). For "pmf", it should contain categorical values such as "low", "moderate", "high", and "very high".

The forecast_data and oracle_output_data must have the same task ID columns and output_type, including output_type_id if necessary, which are used to match the predictions with the ground truth data. As aforementioned, these data frames should follow the model output format and the oracle output format, respectively, as defined by the hubverse convention.

The ensemble_fun argument specifies the ensemble method to be used for evaluating model importance. The currently supported methods are "simple_ensemble" and "linear_pool". The "simple_ensemble" method returns the average of the predicted values from all component models per prediction task defined by task IDs, output_type, and output_type_id columns. The default aggregation function for this method is "mean", but it can be customized by specifying additional arguments through ..., such as agg_fun="median". When "linear_pool" is specified, ensemble model outputs are created as a linear pool of component model outputs. This method supports only an output_type of "mean", "quantile", or "pmf".

The weighted argument is a logical value that indicates whether model weighting should be done when building an ensemble using the specified ensemble_fun. If it is set to TRUE, model weights are estimated based on the previous performance of each model, and these weights are used to build the ensemble.

The importance_algorithm argument specifies the algorithm for model importance calculation, which can be either "lomo" (leave-one-model-out) and "lasomo" (leave all subsets of models out). The subset_wt argument is employed only for the "lasomo" algorithm. This argument has two options: "equal" assigns equal weight to all subsets and "perm based" assigns weight averaged over all possible permutations as in the formula of Shapley values (Algorithm 2). The default values of importance_algorithm and subset_wt are "lomo" and "equal", respectively.

The na action argument allows for specifying how to handle missing values in the forecast_data. Three options are available: "worst", "average", and "drop". In each specific prediction task, if a model has any missing predictions, the "worst" option replaces those missing values with the smallest value from the other models, while the "average" option replaces them with the average of the other models' predictions in that task. The "drop" option removes missing values, which results in the exclusion of the model from the evaluation for that task.

5. Examples

The examples in this section illustrate the use of the model_importance() function to evaluate the importance of component models within an ensemble, using various combinations of the arguments described in Section 4.

5.1. Evaluation using untrained ensemble in LOMO algorithm for mean forecasts

> forecast_data

# 1	A tibble:	10 x 9							
	model_id	reference_date	taı	get			${\tt horizon}$	${\tt location}$	target_end_date
	<chr></chr>	<date></date>	<cl< td=""><td>ır></td><td></td><td></td><td><int></int></td><td><chr></chr></td><td><date></date></td></cl<>	ır>			<int></int>	<chr></chr>	<date></date>
1	model A	2022-11-19	wk	${\tt inc}$	flu	hosp	1	25	2022-11-26
2	model A	2022-11-19	wk	${\tt inc}$	flu	hosp	3	25	2022-12-10
3	model A	2022-11-19	wk	${\tt inc}$	flu	hosp	1	48	2022-11-26
4	model A	2022-11-19	wk	${\tt inc}$	flu	hosp	3	48	2022-12-10
5	model B	2022-11-19	wk	${\tt inc}$	flu	hosp	3	25	2022-12-10
6	model B	2022-11-19	wk	${\tt inc}$	flu	hosp	1	48	2022-11-26
7	model B	2022-11-19	wk	${\tt inc}$	flu	hosp	3	48	2022-12-10
8	${\tt model}\ {\tt C}$	2022-11-19	wk	${\tt inc}$	flu	hosp	1	25	2022-11-26
9	model C	2022-11-19	wk	${\tt inc}$	flu	hosp	3	25	2022-12-10
10	model C	2022-11-19	wk	inc	flu	hosp	1	48	2022-11-26
	output_type output_type_id value								
	<chr></chr>	<chr></chr>		<db1< td=""><td>L></td><td></td><td></td><td></td><td></td></db1<>	L>				
1	mean	<na></na>		Ę	51				
2	mean	<na></na>		į	53				

3	mean	<na></na>	21
4	mean	<na></na>	21
5	mean	<na></na>	47
6	mean	<na></na>	21
7	mean	<na></na>	14
8	mean	<na></na>	92
9	mean	<na></na>	3
10	mean	<na></na>	24

- 5.2. Evaluation using untrained ensemble in LASOMO algorithm for quantile-based forecasts
- 5.3. Evaluation using trained ensemble in LOMO algorithm for quantile-based forecasts

TO DO

5.4. Evaluation using trained ensemble in LOMO algorithm for mean forecasts

TO DO

6. Summary and discussion

Multi-model ensemble forecasts often provide better accuracy and robustness than single models, and are widely used in decision-making and policy planning across various domains. The contribution of each component model to the accuracy of the ensemble depends on its own unique characteristics. The **modelimportance** package enables the quantification of the value that each component model adds to the ensemble performance in different evaluation contexts.

The primary function of the package is model_importance(), which returns a data frame with component models and their importance metrics. It allows users to choose the ensemble approach and model importance algorithm, selecting between LOMO and LASOMO. Additionally, it provides customizable options for handling missing values. These features enable the package to serve as a versatile tool to aid collaborative efforts to construct an effective ensemble model across a wide range of forecasting tasks.

There is a room to enhance the current version of this package.

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These extensions would aim to broaden the scope of applications in real-world forecasting tasks.

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Submitted: yyyy-mm-dd

Accepted: yyyy-mm-dd