FLEXIBLE MODEL COMPOSITION IN MACHINE LEARNING
AND ITS IMPLEMENTATION IN MLJ

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Abstract. A graph-based protocol called ‘learning networks’ which combine assorted machine learning models into meta-models is described. Learning networks are shown to overcome several limitations of model composition as implemented in the dominant machine learning platforms. After illustrating the protocol in simple examples, a concise syntax for specifying a learning network, implemented in the MLJ framework, is presented. Using the syntax, it is shown that learning networks are sufficiently flexible to include Wolpert’s model stacking, with out-of-sample predictions for the base learners.

1. Introduction

This paper details a general scheme for composing machine learning models, implemented in the open-source machine learning toolbox MLJ (Machine Learning in Julia) but likely to be of interest more generally [2]. The paper [4] gives an overview of MLJ’s design without providing the detail on model composition, which is this paper’s exclusive focus.

An increasingly essential feature of a machine learning toolbox is a facility for combining basic machine learning elements into more sophisticated meta-models. The earliest example of such model composition is the simple non-branching pipeline. A pipeline model typically combines, in sequence, several pre-processing operations — such as type coercion and missing-value imputation — with a final supervised learning model. It seems pipelines were first popularized by the scikit-learn toolbox [11] [6].

Another early example of a composite model is the homogeneous ensemble. Here the predictions of a large number of simple atomic learners are aggregated; each is trained with the same algorithm and each learner shares the same hyperparameters, but incorporates some random element to increase variance. The most well-known example of this is the random forest, whose atomic elements are decision trees [5].

Inhomogeneous ensembles, blending the predictions of a relatively small number of different but sophisticated models has also been shown to improve performance. The most advanced model composition of this kind is known as model stacking [12] and is used routinely by winning teams of data science competitions, such as kaggle.

However, several limitations surrounding model composition are increasingly evident to users of the dominant machine learning software platforms, which were
not developed with flexible model composition in mind. For instance, the basic model composition interfaces provided by \texttt{mlr} \cite{Bischl10}, \texttt{caret} \cite{Lawrence2012}, \texttt{sckit-learn} \cite{Pedregosa11, Blaom17}, and \texttt{Weka} \cite{Witten2016} all share one or more of the following shortcomings:

1. Composite models do not inherit all the behavior of ordinary models.
2. Composition is limited to linear (non-branching) pipelines.
3. Supervised components in a linear pipeline can only occur at the end of the pipeline.
4. Only static (unlearned) target transformations / inverse transformations are supported.
5. Hyper-parameters in homogeneous model ensembles cannot be coupled.
6. Some sophisticated inhomogeneous ensembling, such as stacking (with out-of-sample predictions for base learners) cannot be implemented.
7. Composite models cannot implement multiple operations, for example, both a ‘predict’ and ‘transform’ method (as in clustering models) or both a ‘transform’ and ‘inverse transform’ method.

The purpose of this article is to: (i) outline a model composition scheme flexible enough to mitigate the above shortcomings; and (ii) describe a model composition syntax adopted in \texttt{MLJ} which implements the proposed scheme.

The design of \texttt{MLJ} is partly inspired by that of \texttt{mlr}. The latter package’s reincarnation \texttt{mlr3}, developed concurrently, also overcomes the obstacles mentioned above, with exception of (4) \cite{Bischl19}. The approach taken there is not the same, however.

1.1. \textbf{Sources of current design limitations}. Composite machine learning models are generally conceived as some kind of directed acyclic graph structure $G$, whose nodes are the component models. In our assessment, existing design limitations arise from two common design decisions:

Firstly, a given node is associated simultaneously with a unique set of hyper-parameters, a corresponding set of learned parameters, and a single operation, such as ‘predict’ or ‘transform’. However, in the case of pipeline target transformations, for example, you want two nodes with different operations (transform and inverse transform) but which point to the same learned parameters. In a homogeneous ensemble, you want multiple nodes pointing to the same model hyper-parameters, but enjoying distinct learned parameters.

Secondly, there may be an implicit requirement that the same graph structure essentially reflect both the flow of information during training as in prediction. An example where this is too restrictive is model stacking \cite{Wager17}, where: (i) each base learner computes multiple sets of learned parameters, one set for each fold of the provided data, to obtain an out-of-sample base-learner prediction, used to train the adjudicator; but (ii) the adjudicating model looks to base model nodes trained on all the training data when predicting on new data.

1.2. \textbf{The main idea}. In our conception a \textit{node} is just some object that can be called upon to deliver data, lazily computed in some way. To separate the various
objects conflated in existing designs, it is convenient to introduce one mild abstraction, which we call a machine. A machine is an object pointing to a set of model hyperparameters $h$ (the model) and a sequence of nodes $N_1, N_2, ..., N_k$ (the arguments) from a base graph $G$. These nodes indicate where the model should look for its training data. In training, a single set of learned parameters is associated with each machine.

A composite model is then specified by specifying the underlying graph $G$ and by labeling certain nodes — called dynamic — with machines and corresponding operations (such as predict or inverse transform), and certain other nodes — called static — with ordinary functions. Training a dynamic node means training the machine that labels it (i.e., training the model specified by the machine). To train the composite model as a whole, machines must be individually trained in an appropriate order. The labeled graph is called a learning network.

We re-iterate that the learned parameters of training a machine are always associated with the machine and not with any particular node or model. Two nodes can be labeled with the same machine (but different operations) and we allow distinction between two machines with identical model and node specification.

Our idea is clarified in a simple example presented in 2.2.

Learning networks are described in Section 2, which includes some simple examples. Section 3 introduces a concise syntax for specifying a learning network, implemented in MLJ, and goes on to show how Wolpert’s model stacking can be implemented.

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2. A FORMAL SPECIFICATION FOR MODEL COMPOSITION

2.1. Learners. To train a decision tree requires the specification of hyper-parameters, such as the maximum tree depth. Such a specification (algorithm + hyper-parameters) is here called a model (also known as a hypothesis or learning strategy). The learning algorithm itself will be understood as a family of fitting functions $f_h(X, y) \in \Theta$, one for each model $h$. Here $\Theta$ is the space of all possible decision trees, which we more generally refer to as learned parameters. Here $X$ and $y$ are feature observations and target observations for training the decision tree.

Once a learned parameter (tree) $\theta = f_h(X, y)$ is computed, predictions for new feature observations $X'$ are given by $p(\theta, X')$, for some function $p$, the prediction operation.

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1Even ‘non-deterministic’ algorithms, such as random forests, can be viewed as functions if we regard the random number generator seed as a hyper-parameter.
A decision tree is an example of a learner. More generally, we are interested in forming new learners by combining (composing) a number of existing learners, where, in general, a learner consists of:

1. a set $H$ of models, each trained using the using the same algorithm
2. a set $\Theta$ of learned parameters
3. fitting functions $(X_1, X_2, \ldots, X_{k_H}) \mapsto f_h(X_1, X_2, \ldots, X_{k_H}) \in \Theta$, one for each $h \in H$; and
4. one or more operations of the form $p: \Theta \times X_p \rightarrow Y_p$

The variables $X_1, X_2, \ldots, X_{k_H}$ are called training arguments.

The learner is unsupervised if $k_H = 1$ and there exists an operation $t: \Theta \times X_t \rightarrow Y_t$, called the transformation operation, subject to the understanding that $X_1$ is always drawn from $X_t$. Some unsupervised learners will have an inversion operation $i$, with the property that $i(\theta, \cdot)$ and $t(\theta, \cdot)$ are inverses (or approximately so).

The learner is supervised if $k_H \geq 2$ and there exists an operation $p: \Theta \times X_p \rightarrow Y_p$, called the prediction operation such that $X_1$ is drawn from $X_p$ and $X_2$ from $Y_p$. (A third argument $X_3$ of the fitting functions might represent, for example, sample weights, for supervised learners that support them.)

2.2. A simple example of a learning network. A composite learner is one whose fitting functions and operations are encoded in a certain directed graph, here called a learning network, labeled with metadata pertaining to the learners to be composed.

Before stating the definition of learning networks, we informally describe the example illustrated in Figure 1. This combines an ordinary supervised learner $h_S$, with prediction $p_S$, and a learned transformation of the target $h_T$, with transformation $t_T$ and inverse $i_T$. Specifically: (i) The network learns a target transformation (such as normalization) using training data supplied at $y$; (ii) the supervised model is trained using features supplied at $X$, together with the transformed training target fetched from $z$; (iii) the network outputs at $\hat{z}$ the predictions of the supervised model, on new features to be supplied at $X$; and (iv) applies the inverse of the target transformation learned in (i) to the predictions at $\hat{z}$ to obtain the final output $\hat{y}$ (restoring the original target scale, in the example of normalization).

Observe that each non-source node is labeled with both an operation — $p_S$, $i_T$, or $t_T$ — and tuple, such as $(2, h_T, y)$, called a machine. The operation indicates how the node should process incoming information, while the machine refers to a training event on which the operation depends. For example, the node $\hat{y}$ applies the inverse transform $i_T$ to incoming data, using the parameter $\theta$ learned by fitting the model $h_T$ to data fetched from the source node $y$. The node $z$ similarly depends on the same training event (machine) and so receives the same machine as label. The first number in the machine is purely an identifier. (Two machines could specify the same model and nodes, but would be distinct, and hence be associated with distinct learned parameters, if their identifiers are different.)
2.3. Machines and learning networks defined. Let $G$ be a graph. Then a machine over $G$ is any tuple of the form $m = (i, h, N_1, N_2, \ldots, N_k)$, where $i$ is an integer (the identifier), $h$ is a model associated with some learner $L$ having $k$ training arguments, and $N_1, N_2, \ldots, N_k$ are nodes of $G$ (the machine training arguments). We call $L$ the learner of $m$. The learning network above has exactly two machines (one of which happens to label two different nodes).

Formally, a learning network consists of:

1. a finite, directed, simple, acyclic graph $G$, subject to the restriction that each connected component of $G$ has a unique source node
2. an enumeration of the set of incoming edges of any non-source node $N$ of $G$, or, equivalently, an enumeration $N^1, N^2, \ldots, N^{k_N}$ of those nodes with an outgoing edge ending at $N$
3. an enumeration $S^1, S^2, \ldots, S^{k_S}$ of the set of source nodes
4. a declaration of each non-source node of $N \in G$ as static or dynamic such that dynamic nodes have unique incoming edges
5. a labeling of each static node $N \in G$ with a function $(X_1, X_2, \ldots, X_{k_N}) \mapsto p_N(X_1, X_2, \ldots, X_{k_N})$, where $k_N$ is the number of incoming edges
6. a finite sequence of machines $m_1, m_2, \ldots, m_R$ of machines over $G$, such that $m_j$ has identifier $j$
7. a labeling of each dynamic node $N \in G$ with: (i) an integer $j$ representing the identifier of one of the machines; and (ii) an operation $p_N$ for the learner of the machine labeling $N$
8. for each operation $p$ that the corresponding composite learner is to support, a declaration of some node $N(p)$.
Elaborating on the last requirement, if, for example, the composite model defined by the network is be considered a supervised model, with a single predict operation, then the corresponding node indicates where predictions are to be fetched.

Note that the same machine may label distinct dynamic nodes, and two machines may specify the same model and/or training nodes.

All non-source nodes in the simple target transformation example of the previous section (Figure 1) have a single incoming edge, but there is no static node.

The learning network shown in Figure 2 specifies a homogeneous ensemble of a three supervised learners whose predictions are to be aggregated. Each dynamic node \( \hat{y}_1, \hat{y}_2 \) and \( \hat{y}_3 \) is labeled with a separate machine (and so will predict using a separate learned parameter). However, as each machine specifies the same model \( h \), the model hyper-parameters are coupled (as the tree parameters in a random forest). The node \( \hat{y} \) is static and its static operation (function) \( \mu \) represents aggregation (e.g., “compute mean” in the case \( h \) is a regressor).

- **Figure 2.** A three-model homogeneous ensemble with atomic model \( h \), which is shared by the three distinct machines labeling the nodes \( \hat{y}_1, \hat{y}_2, \hat{y}_3 \). Predictions are aggregated using the function \( \mu \) at node \( \hat{y} \).

A learning network for model stacking is described in Section 3.

### 2.4. The completion of a learning network.

The underlying graph \( G \) in any learning network may be enlarged to a graph \( \bar{G} \), here called the completion of \( G \), by adding a training edge between nodes \( N \) and \( J \) whenever \( N \) appears as a training argument of a machine labeling \( J \). The training edges in learning network of Figure 2 are shown as dashed arrows in Figure 3. The complication of the completed network, even in this simple and common use-case, highlights the subtlety of model composition in machine learning.
When one applies an operation to a learning network — for example, calls on the supervised learning network in Figure 3 to make a prediction — then the training edges play no role. However, as we detail in 2.5, training a learning network means training its machines, and training a machine means calling on its training arguments to deliver training data. In this case one may imagine data flowing along the training edges, with the following caveat: Since the same machine may label multiple nodes ($z$ and $\hat{y}$ in the figure are labeled by the same machine) distinct training edges may actually represent the same data flow (e.g., $\alpha$ and $\beta$).

The main significance of the graph $\bar{G}$ is that encodes dependencies. A machine $m$ labeling a node $N$ is ready to be trained when all machines labeling nodes upstream of $N$ in $\bar{G}$ are already trained.

2.5. The composite learner defined by a learning network. The magnanimous reader will likely guess at the manner in which a learning network $G$ can be interpreted as a new composite learner $L$ without detailed explanation. However, for completeness, and to mitigate any ambiguity, we provide details below.

Our main goal is to describe the fitting function of the composite learner. For conceptual simplicity, we describe this function in a rather naive way; in the MLJ implementation component models are trained asynchronously but this detail is not addressed here.

After removing duplicates, we can associate with the machines $m_1, m_2, \ldots, m_R$ of the learning network $G$, a possibly shorter sequence of unique models $h_1, h_2, \ldots, h_R$, drawn from sets of models $H_1, H_2, \ldots, H_r$. By definition, the set of models associated with $L$ is the Cartesian product $H = H_1 \times H_2 \times \cdots \times H_r$. The set of learned parameters of $L$ is defined by $\Theta = \Theta_1 \times \Theta_2 \times \cdots \Theta_R$, where $\Theta_i$ is the set of learned parameters for the learner associated with machine $m_i$. So while there may be fewer factors in the set of models than machines, there is exactly one factor in the space of learned parameters for each machine.

We now describe the fitting function for $L$. 

![Figure 3. The learning network of Figure 2.2 with training edges added (shown as dotted arrows).](image)
Suppose we are given training data \( X_1, X_2, \ldots, X_k \), where \( k \) is the number of source nodes. We will simultaneously define learned parameters \( \theta_i \in \Theta_i \) to be associated with each machine \( m_i \), and data, denoted \( N() \), to be associated with the output of each node \( N \) of \( G \).

First, let \( N_1, N_2, \ldots, N_K \) be any enumeration of the nodes of \( G \) consistent with the partial ordering of the directed acyclic graph \( \bar{G} \). That is, if \( N_i \) is upstream of \( N_j \) in \( \bar{G} \), then \( i < j \). From the list of corresponding machine labels, drop any machine with an identical predecessor, obtaining a unique list of machines. Relabeling if necessary, we may assume, without loss of generality, that this list is precisely \( m_1, m_2, \ldots, m_R \). This ordering of machines ensures that the following definition of \( \theta_j \), inductive on index \( j \), is valid:

\[
\theta_j = f_{h_j}(N_{1j}(), N_{2j}(), \ldots, N_{kj}()),
\]

where \( h_j \) is the model associated with \( m_j \), \( N_{1j}, N_{2j}, \ldots, N_{kj} \) are the training arguments of \( m_j \), and where the definition of \( N() \), for each \( N \in \{N_{1j}, N_{2j}, \ldots, N_{kj}\} \), depends on whether \( N \) is dynamic, static, or a source node, as follows.

If \( N \) is dynamic, then

(1) \( N() = p_N(J(), \mu) \),

where \( J \) is the (unique) input node of \( N \), and \( \mu \) the learned parameter associated with the machine labeling \( N \). If \( N \) is static, then instead,

(2) \( N() = p_N(J_1(), J_2(), \ldots, J_l()) \),

where \( J_1, J_2, \ldots, J_l \) are the input nodes of \( N \). If \( J \) is a source node, then

(3) \( N() = X_i \),

where \( i \) is the index of \( N \) in the prescribed enumeration of source nodes.

With \( \theta_1, \theta_2, \ldots, \theta_R \) so defined, the fitting function for \( L \) is

\[
f(\theta_1, \ldots, \theta_R)(X_1, X_2, \ldots, X_k) = (\theta_1, \theta_2, \ldots, \theta_R)
\]

Having defined training, let us finish by explaining how the network operates in ‘prediction’ mode. That is, we need to define the map \( p: \Theta \times X_p \rightarrow Y_p \) for each operation \( p \) to be defined for the composite model. To this end, we extend the recursive definitions [1]–[3] to allow calling a node with a single argument \( X' \):

\[
N(X') = p_N(J(X'), \mu) \quad \text{if } N \text{ is dynamic}
\]

\[
N(X') = p_N(J_1(X'), J_2(X'), \ldots, J_l(X')) \quad \text{if } N \text{ is static}
\]

\[
N(X') = X' \quad \text{if } N \text{ is a source node}
\]

Then the new operations are defined by \( p(\theta_1, \ldots, \theta_R, X') = N(p)(X') \), where \( N(p) \) is the node declared in condition 2.3[8].
3. An advanced application: model stacking

We now introduce the syntax used in MLJ for defining a learning network, and demonstrate how model stacking can be implemented using such a syntax. A pictorial description of the underlying graph is probably too complicated here to be immediately useful, and we do not attempt to provide one.

Because Julia foregoes abstractions such as classes in favor of a more functional paradigm, this syntax is close to the mathematical description given already, and familiarity with Julia will not be necessary to understand what follows.

3.1. A syntax for learning networks. Recall once again that a model is just a set of hyperparameters for some machine learning algorithm (in MLJ, an instance of a composite type). A machine, as defined in [2,3] is an object pointing to some model and some training arguments (nodes), and is constructed in MLJ with the syntax

\[
\text{mach} = \text{machine}(\text{model}, \text{arg1}, \text{arg2}, \ldots)
\]

This object, which is mutable, additionally stores learned parameters after training.\footnote{In Julia the mutability has the consequence that the machine identifiers referred to earlier are redundant — a second machine constructed with the same call will be considered a distinct object.}

A source node is constructed with the syntax \(X = \text{source}()\) and a new node is generated in one of two ways:

1. To generate a dynamic node labeled with machine \(\text{mach}\) and a given operation — such as predict or transform — we call the operation on the machine and the node that is to be the parent of that node (always unique). For example, we might declare \(\text{yhat} = \text{predict}(\text{mach}, X)\). In this case, when called on to do so, the new node \(\text{yhat}\) fetches feature data from node \(X\) and determines the prediction using learned parameters stored at \(\text{mach}\).
2. To generate a static node, a function that ordinarily takes data as arguments (vectors, tables, etc) is simply overloaded to act on nodes, with a node as return value. In MLJ this can be done using a macro, but here we shall tacitly assume all functions have already been overloaded in this way. So, for example, if \(y_1\) and \(y_2\) are two nodes for delivering equi-length vector data, then \(y_1 + y_2\) is a new static node which, when called to do so, fetches data from nodes \(y_1\) and \(y_2\) and adds the result. Similarly, \(z = \text{mean}(y_1)\) defines a new node \(z\) that computes the mean of data fetched from \(y_1\).

To illustrate (1), consider again the learning network depicted in Figure 2, for wrapping a supervised learner in a target transformation / inverse transformation. For concreteness, suppose the supervised learner \(h_S\) is a decision tree regressor, and the target transformer \(h_T\) is a standardizer (whitener). Then the following is valid MLJ code defining the composite learning network:
# load necessary libraries:
using MLJ
@load DecisionTreeRegressor

# instantiate model instances:
tree = DecisionTreeRegressor(min_samples_split=5)
standardizer = Standardizer()

X = source()
y = source()

# the machine (2, h_T, y):
mach2 = machine(standardizer, y)

z = transform(mach2, y)

# the machine (1, h_S, X, z):
mach1 = machine(tree, X, z)

zhat = predict(mach1, X)
yhat = inverse_transform(mach2, zhat)

In MLJ a learning network can be ‘exported’ to define a new re-usable, stand-alone model type, whose fields are commonly the component models (tree and standardizer in the example above) and these can be mutated. For details, the reader is referred to the ‘Composing Models’ section of the MLJ documentation [3].

3.2. Model stacking. David Wolpert describes a rather general method for blending the predictions of multiple models known as model stacking [12]. A basic two-layer stack consists of a number of base learners and a single adjudicating learner. When such a stack is called to make a prediction, the individual predictions of the base learners are made the columns of a feature table for the adjudicating learner, which then outputs the final prediction. However, it is crucial to understand that the flow of data during training is not the same.

The base model predictions used to train the adjudicating model are not the predictions of the base learners fitted to all the training data. Rather, to prevent the adjudicator giving too much weight to the base learners with low training error, the input data is first split into a number of folds (as in cross-validation). A base learner is then trained on each fold complement individually, and corresponding predictions on the folds are spliced together to form a full-length prediction called an out-of-sample prediction. It is these out-of-sample predictions that are used to train the adjudicating model.

For readability, we limit our stacking illustration to two base learners, with three folds for the out-of-sample predictions. Each base learner will get three separate
machines, for training on each fold complement, and a fourth machine, trained
on all the supplied data, for use in the prediction flow. Then there is one more
machine for training the adjudicator. Our code snippet makes use of the following
functions, assumed to have been overloaded to admit nodes as arguments:

- \texttt{folds}(X, n): Return an \(n\)-tuple of vectors of indices, as if for use in \(n\)-fold
cross-validation. For example, if \(X\) is a table with ten rows, then \texttt{folds}(X,
\(n\)) returns \([1, 2, 3], [4, 5, 6], [7, 8, 9, 10]\).
- \texttt{restrict}(X, folds, i): Return the restriction of data object \(X\) to the
\(i\)th fold of \texttt{folds}.
- \texttt{corestrict}(X, folds, i): Return the restriction of data object \(X\) to the
complement of the \(i\)th fold of \texttt{folds},
- \texttt{vcat, hcat} — vertical and horizontal concatenation
- \texttt{MLJBase.table} — operation converting a matrix to a table

For concreteness, we suppose the base models are a gradient tree booster and a
support vector machine; the adjudicator is a random forest:

```julia
@load EvoTreesRegressor
@load SVMRegressor;
@load RandomForestRegressor pkg=DecisionTree

model1 = EvoTreesRegressor(nrounds=100)
model2 = SVMRegressor()
judge = RandomForestRegressor(n_trees=500)

X = source()
y = source()

f = folds(X, 3) # a node!

# for training model1 on each fold complement:
m11 = machine(model1, corestrict(X, f, 1), corestrict(y, f, 1))
m12 = machine(model1, corestrict(X, f, 2), corestrict(y, f, 2))
m13 = machine(model1, corestrict(X, f, 3), corestrict(y, f, 3))

# predictions for model1 on each fold:
y11 = predict(m11, restrict(X, f, 1));
y12 = predict(m12, restrict(X, f, 2));
y13 = predict(m13, restrict(X, f, 3));

# for training model2 on each fold complement:
m21 = machine(model2, corestrict(X, f, 1), corestrict(y, f, 1))
m22 = machine(model2, corestrict(X, f, 2), corestrict(y, f, 2))
m23 = machine(model2, corestrict(X, f, 3), corestrict(y, f, 3))

# predictions for model2 on each fold:
```
y21 = predict(m21, restrict(X, f, 1));
y22 = predict(m22, restrict(X, f, 2));
y23 = predict(m23, restrict(X, f, 3));

# the out-of-sample predictions for base learners:
y1_oos = vcat(y11, y12, y13);
y2_oos = vcat(y21, y22, y23);

# make out-of-sample predictions columns of a table:
X_oos = MLJ.table(hcat(y1_oos, y2_oos))

# for training the adjudicator:
m_judge = machine(judge, X_oos, y)

# for training the base models on all available data:
m1 = machine(model1, X, y)
m2 = machine(model2, X, y)

# for processing *new* input features for feeding to the adjudicator:
y1 = predict(m1, X);
y2 = predict(m2, X)

# assembling the base-learner predictions on the new inputs:
X_judge = MLJ.table(hcat(y1, y2))

# for outputing the final prediction on new inputs:
yhat = predict(m_judge, X_judge)

For complete MLJ code for this example, see the Stacking tutorial at [10].

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