

Package ‘ROOT’

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Title ROOT (Rashomon Set of Optimal Trees)

Version 0.0.0.9000

Description ROOT (Rashomon Set of Optimal Trees) is a general framework for globally optimizing user-specified objective functionals over interpretable binary weight functions represented as sparse decision trees. It searches over candidate trees to construct a Rashomon set of near-optimal solutions and derives a summary tree highlighting stable patterns in the optimized weights. ROOT includes a built-in generalizability mode for identifying subgroups in trial settings for transportability analyses.

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characterizing_underrep

Characterize Underrepresented Subgroups

Description

A high-level wrapper around `ROOT()` for identifying and characterizing subgroups that are *insufficiently represented* in a randomized controlled trial (RCT) relative to a target population. The function returns an interpretable decision tree describing which subgroups should be included ($w(X) = 1$) or excluded ($w(X) = 0$) from the analysis, along with the corresponding target treatment average effect estimates.

Usage

```
characterizing_underrep(
  data,
  global_objective_fn = NULL,
  generalizability_path = FALSE,
  leaf_proba = 0.25,
  seed = 123,
  num_trees = 10,
  vote_threshold = 2/3,
  explore_proba = 0.05,
  feature_est = "Ridge",
  feature_est_args = list(),
  top_k_trees = FALSE,
  k = 10,
  cutoff = "baseline",
  verbose = FALSE
)
```

Arguments

<code>data</code>	A <code>data.frame</code> containing covariates and, in generalizability mode, also columns <code>Y</code> , <code>Tr</code> , and <code>S</code> .
<code>global_objective_fn</code>	A function with signature <code>function(D) -> numeric</code> scoring the entire state and minimized by <code>ROOT</code> . If <code>NULL</code> (the default), a variance-based objective is used that targets the precision of the WTATE estimator.
<code>generalizability_path</code>	Logical. If <code>TRUE</code> , runs the full generalizability analysis (design + analysis stages) and expects columns <code>Y</code> , <code>Tr</code> , and <code>S</code> in <code>data</code> . If <code>FALSE</code> , runs <code>ROOT</code> in general optimization mode. Default <code>FALSE</code> .

leaf_proba	A numeric(1) tuning parameter that increases the chance a node stops splitting by selecting a synthetic "leaf" feature. Internally, the probability of choosing "leaf" is $\text{leaf_proba} / (1 + \text{leaf_proba})$ (assuming the covariate probabilities sum to 1). Higher values produce shallower, more interpretable trees. Default 0.25.
seed	Random seed for reproducibility.
num_trees	Number of trees to grow in the ROOT forest. More trees explore the tree space more thoroughly but increase computation time.
vote_threshold	Controls how Rashomon-set tree votes are aggregated into w_{opt} . Accepts a numeric threshold in $(0, 1]$, one of "majority" / "mean" / "median", or a custom function(votes) -> integer vector. See ROOT for full details. Default 2/3 (majority vote).
explore_proba	Exploration probability in tree growth. Controls the explore-exploit trade-off: with probability explore_proba , a leaf is assigned a random weight; otherwise, it receives the greedy optimal weight. Default 0.05.
feature_est	Either "Ridge", "GBM", or a custom feature importance function. Used to bias which covariates are selected for splitting. Default "Ridge".
feature_est_args	List of extra arguments passed to <code>feature_est</code> when it is a function.
top_k_trees	Logical; if TRUE, selects the top k trees by objective value for the Rashomon set. If FALSE, uses cutoff instead. Default FALSE.
k	Number of trees to retain when <code>top_k_trees</code> = TRUE. Default 10.
cutoff	Numeric or "baseline". When <code>top_k_trees</code> = FALSE, trees with objective values below this cutoff are included in the Rashomon set. "baseline" uses the objective value at $w \equiv 1$ (no subgroups excluded). Default "baseline".
verbose	Logical; if TRUE, prints the unweighted and weighted estimands with standard errors. Default FALSE.

Value

A `characterizing_underrep` S3 object (a list) with:

root	The ROOT object returned by <code>ROOT()</code> . Contains the Rashomon set, weight assignments (<code>root\$D_rash\$w_opt</code>), summary tree (<code>root\$f</code>), and (in generalizability mode) treatment effect estimates (<code>root\$estimate</code>).
combined	The input data.
leaf_summary	A <code>data.frame</code> with one row per terminal node of the summary (characteristic) tree, giving the decision rule, predicted weight, sample size, and a label indicating whether the subgroup is "Represented (keep, $w = 1$)" or "Under-represented (drop, $w = 0$)". NULL if no summary tree was produced.

What does "underrepresented" mean?

In the context of generalizing treatment effects from a trial to a target population, a subgroup is considered **underrepresented** (or *insufficiently represented*) when it occupies a region of the covariate space that both (a) has limited overlap between the trial and the target population, and (b) exhibits heterogeneous treatment effects.

Formally, the contribution of a unit with covariates $X = x$ to the variance of the target average treatment effect (TATE) estimator depends on both the selection ratio $\ell(x) = P(S = 1 \mid X =$

$x)/P(S = 0 \mid X = x)$ and the conditional average treatment effect. Subgroups where $\ell(x)$ is small, and conditional average treatment effect deviates from the overall TATE, contribute disproportionately to estimator variance. These are the subgroups that `characterizing_underrep()` identifies and characterizes. The sample average treatment effect (SATE) is a finite sample equivalent version of the TATE.

The generalizability workflow

When `generalizability_path = TRUE`, this function implements the two-stage approach of Parikh et al. (2025):

1. **Design stage:** ROOT learns binary weights $w(X)$ that minimize the variance of the weighted target average treatment effect (WTATE) estimator, subject to interpretability constraints (tree structure). The resulting decision tree characterizes which subgroups are well-represented ($w = 1$) and which are underrepresented ($w = 0$).
2. **Analysis stage:** The WTATE is estimated on the refined target population that excludes the underrepresented subgroups. This estimand trades some generality for greater precision and credibility.

The key estimands are:

- **SATE** (Sample Average Treatment Effect): the treatment effect for the full target population based on the trial sample, which may be imprecise if certain subgroups are underrepresented. It is a finite sample equivalent version of the TATE.
- **WTATE** (Weighted Target Average Treatment Effect): the treatment effect restricted to the sufficiently represented subpopulation, estimated with lower variance.

General optimization mode

When `generalizability_path = FALSE`, this function behaves as a convenience wrapper around `ROOT()` for arbitrary binary weight optimization. The user can supply a custom objective function via `global_objective_fn`; ROOT will learn an interpretable tree-based weight function minimizing that objective. See `vignette("optimization_path_example")` for an example.

Data requirements

When `generalizability_path = TRUE`, data must contain the following standardized columns:

- Y: numeric outcome variable.
- Tr: binary treatment indicator (0 = control, 1 = treated).
- S: binary sample indicator (1 = trial/RCT, 0 = target population).

All remaining columns are treated as pretreatment covariates X available for splitting.

References

Parikh H, Ross RK, Stuart E, Rudolph KE (2025). "Who Are We Missing?: A Principled Approach to Characterizing the Underrepresented Population." *Journal of the American Statistical Association*. doi:10.1080/01621459.2025.2495319

See Also

`ROOT` for the underlying optimization engine; `vignette("generalizability_path_example")` for a detailed worked example of the generalizability workflow; `vignette("optimization_path_example")` for general optimization mode.

Examples

```
## Not run:
# --- Generalizability analysis ---
# diabetes_data has columns Y, Tr, S, and covariates
data(diabetes_data, package = "ROOT")

char_fit <- characterizing_underrep(
  data = diabetes_data,
  generalizability_path = TRUE,
  num_trees = 20,
  top_k_trees = TRUE,
  k = 10,
  seed = 123
)

# View the characterization tree
plot(char_fit)

# Inspect which subgroups are underrepresented
char_fit$leaf_summary

# Treatment effect estimates (SATE and WTATE)
char_fit$root$estimate

## End(Not run)
```

diabetes_data	<i>Simulated diabetes dataset for examples</i>
---------------	--

Description

A toy dataset for illustrating ROOT examples and tests.

Usage

```
data(diabetes_data)
```

Format

A `data.frame` with one row per individual and the columns:

Age45 Indicator in 0/1: age ≥ 45 .

DietYes Indicator in 0/1: on a diet program.

Race_Black Indicator in 0/1: race is Black.

S Sample indicator in 0/1: 1 means RCT or source, 0 means target.

Sex_Male Indicator in 0/1: male.

Tr Treatment assignment in 0/1.

Y Observed outcome (numeric or 0/1).

plot.characterizing_underrep

Plot Under represented Population Characterization

Description

Visualizes the decision tree derived from the ROOT analysis. Highlights which subgroups are represented where $w = 1$ versus underrepresented where $w = 0$ in generalization mode, or simply $w(x)$ in $\{0, 1\}$ in general optimization mode.

Usage

```
## S3 method for class 'characterizing_underrep'
plot(
  x,
  main = "Final Characterized Tree from Rashomon Set",
  cex.main = 1.2,
  ...
)
```

Arguments

x	A characterizing_underrep S3 object with x\$root\$f present as an rpart object for the summary or characterization tree.
main	Character string for the plot title. Default is "Underrepresented Population Characterization".
cex.main	Numeric scaling factor for the title text size. Default is 1.2.
...	Additional arguments passed to rpart.plot::prp().

Value

NULL. The plot is drawn to the active graphics device.

plot.ROOT

Plot the ROOT summary tree

Description

Visualizes the decision tree that characterizes the weighted subgroup (the weight function $w(d)$ in $\{0, 1\}$) identified by ROOT(), using rpart.plot::prp().

Usage

```
## S3 method for class 'ROOT'
plot(x, ...)
```

Arguments

`x` A "ROOT" S3 object returned by `ROOT()` with `x$f` an `rpart` object representing the summary / characterization tree.

`...` Additional arguments passed to `rpart.plot::prp()`.

Value

No return value; the plot is drawn to the active graphics device.

Examples

```
## Not run:
ROOT.output = ROOT(diabetes_data,generalizability_path = TRUE, seed = 123)
plot(ROOT.output)

## End(Not run)
```

```
print.characterizing_underrep
      Print a characterizing_underrep fit
```

Description

Print the ROOT summary which includes unweighted and (when in generalization mode) weighted estimates with standard errors, as reported by `summary.ROOT()`.

Usage

```
## S3 method for class 'characterizing_underrep'
print(x, ...)
```

Arguments

`x` A `characterizing_underrep` S3 object. Expected components include `root` which is a ROOT object (summarized by `print.ROOT()`) and may contain `f` which is an `rpart` object for the summary tree, and `leaf_summary` which is a `data.frame` with one row per terminal node and may include a `rule` column of type `character`.

`...` Currently unused. Included for S3 compatibility.

Details

Delegates core statistics and estimands to `print(x$root)`.

Value

object returned invisibly. Printed output is a readable brief summary.

Abbreviations

ATE Average treatment effect.
RCT Randomized controlled trial.
SE Standard error.
TATE Transported average treatment effect.
WTATE Weighted transported average treatment effect.
SATE Sample average treatment effect.

Examples

```
## Not run:
char.output = characterizing_underrep(diabetes_data, generalizability_path = TRUE, seed = 123)
print(char.output)

## End(Not run)
```

print.ROOT

Print a ROOT fit

Description

Provides a human-readable brief summary of a ROOT object, including:

1. the summary characterization tree f,
2. in generalizability mode (`generalizability_path = TRUE`), the unweighted and weighted estimands with their standard errors and an explanatory note for the weighted standard error (SE).

Usage

```
## S3 method for class 'ROOT'
print(x, ...)
```

Arguments

`x` A "ROOT" S3 object returned by `ROOT()`.
`...` Currently unused and included for S3 compatibility.

Value

object returned invisibly. Printed output is for inspection.

Abbreviations

ATE Average treatment effect.

RCT Randomized controlled trial.

SE Standard error.

TATE Transported average treatment effect.

WTATE Weighted transported average treatment effect.

SATE Sample average treatment effect.

When `generalizability_path = TRUE`, the unweighted estimand corresponds to a SATE-type quantity and the weighted estimand to a WTATE-type quantity for the transported target population. When `generalizability_path = FALSE`, ROOT is used for general functional optimization and no causal labels are imposed.

Examples

```
## Not run:
ROOT.output = ROOT(diabetes_data, generalizability_path = TRUE, seed = 123)
print(ROOT.output)

## End(Not run)
```

ROOT

Rashomon Set of Optimal Trees (ROOT) for Functional Optimization

Description

ROOT (Rashomon Set of Optimal Trees) is a general-purpose functional optimization algorithm that learns interpretable, tree-structured binary weight functions $w(X) \in \{0, 1\}$. Given a dataset D_n and a global objective function $L(w, D_n)$, ROOT searches over the space of decision trees to find weight assignments that minimize the objective function.

Usage

```
ROOT(
  data,
  global_objective_fn = NULL,
  generalizability_path = FALSE,
  leaf_proba = 0.25,
  seed = NULL,
  num_trees = 10,
  vote_threshold = 2/3,
  explore_proba = 0.05,
  feature_est = "Ridge",
  feature_est_args = list(),
  top_k_trees = FALSE,
  k = 10,
  cutoff = "baseline",
  verbose = FALSE
)
```

Arguments

data	<p>A data.frame containing the dataset.</p> <p>In general optimization mode (<code>generalizability_path = FALSE</code>), data can contain any covariates and auxiliary columns. The user supplies a <code>global_objective_fn</code> that takes a data frame with a column <code>w</code> and returns a scalar loss.</p> <p>In generalizability mode (<code>generalizability_path = TRUE</code>), data must contain columns <code>"Y"</code> (outcome), <code>"Tr"</code> (treatment indicator, 0/1), and <code>"S"</code> (sample indicator, 1 = trial, 0 = target). ROOT internally constructs transportability scores and, if no custom objective is given, uses a default variance-based loss.</p>
global_objective_fn	<p>A function with signature <code>function(D) -> numeric</code> scoring the entire state and minimized by ROOT. <code>D</code> is the working data frame containing at least a column <code>w</code> with the current weight assignments. If <code>NULL</code> (default), a variance-based objective is used.</p>
generalizability_path	<p>Logical(1). If <code>TRUE</code>, use the built-in transportability objective for trial-to-target generalizability. If <code>FALSE</code>, treat data as arbitrary and rely on <code>global_objective_fn</code>. Default <code>FALSE</code>.</p>
leaf_proba	<p>A numeric tuning parameter that increases the chance a node stops splitting by selecting a synthetic "leaf" feature. Internally, the probability of choosing "leaf" is $\text{leaf_proba} / (1 + \text{leaf_proba})$ (assuming the covariate probabilities sum to 1). Higher values produce shallower, sparser trees. Default 0.25.</p>
seed	<p>An optional numeric seed for reproducibility.</p>
num_trees	<p>An integer number of trees to grow. More trees explore the solution space more thoroughly. Default 10.</p>
vote_threshold	<p>Controls how per-observation votes from the Rashomon set trees are aggregated into the final binary weight <code>w_opt</code>. Accepts one of:</p> <ul style="list-style-type: none"> • A numeric in $(0, 1)$: <code>w_opt = 1</code> when the mean fraction of Rashomon-set trees voting 1 strictly exceeds this value. An error is raised if any observation's mean vote equals the threshold exactly (tie is undefined). Default 2/3. • "majority": equivalent to the numeric threshold 2/3. • "mean": <code>w_opt = 1</code> when the mean vote strictly exceeds 0.5. Errors on exact 0.5 ties. • "median": <code>w_opt = 1</code> when the per-row median vote strictly exceeds 0.5. Errors on exact 0.5 ties. • A function with signature <code>function(votes) -> integer vector</code>, where <code>votes</code> is a numeric matrix with one row per observation and one column per Rashomon-set tree (each cell 0 or 1). Must return an integer vector of 0s and 1s of length <code>nrow(votes)</code>.
explore_proba	<p>A numeric giving the exploration probability at leaves. With probability <code>explore_proba</code>, a leaf receives a random weight; otherwise the greedy-optimal weight is used. Default 0.05.</p>
feature_est	<p>Either "Ridge", "GBM", or a custom <code>function(X, y, ...) -> named numeric vector</code> returning nonnegative importance values with names matching columns of <code>X</code>. Used to bias which covariates are chosen for splitting. If the method fails, ROOT falls back to uniform feature sampling with a warning.</p>
feature_est_args	<p>A list of additional arguments passed to a user-supplied <code>feature_est</code> function.</p>

top_k_trees	Logical(1). If TRUE, select the top k trees by objective value for the Rashomon set. If FALSE, use the cutoff threshold. Default FALSE.
k	An integer giving the number of top trees when top_k_trees = TRUE. Default 10.
cutoff	A numeric or "baseline". Used as the Rashomon cutoff when top_k_trees = FALSE. "baseline" uses the objective at $w \equiv 1$ (all weights equal to 1, i.e., no exclusions).
verbose	Logical(1). If TRUE, prints the unweighted and (when available) weighted treatment effect estimates and standard errors in generalizability mode)

Value

An object of class "ROOT" (a list) with elements:

D_rash	Data frame containing the Rashomon-set tree votes and the final aggregated weight w_opt for each observation.
D_forest	Data frame with all forest-level working columns.
w_forest	List of per-tree results from the tree-building routine.
rashomon_set	Integer vector of indices identifying which trees were selected into the Rashomon set.
global_objective_fn	The objective function used.
f	The characteristic (summary) tree fitted to w_opt, as an rpart object. NULL if all observations received the same weight or no covariates were available.
testing_data	Data frame of observations used for optimization (trial units when generalizability_path = TRUE).
estimate	(Only when generalizability_path = TRUE) A list with the unweighted (SATE) and weighted (WTATE) point estimates, standard errors, and a note about the SE calculation.
generalizability_path	Logical flag echoing the input.

The optimization problem

ROOT solves the functional optimization problem:

$$w^* \in \arg \min_w L(D_n, w)$$

where $w : \mathbb{R}^p \rightarrow \{0, 1\}$ maps a p -dimensional covariate vector to a binary include/exclude decision. The key challenge is that, unlike standard tree algorithms, the global loss $L(D_n, w)$ is not decomposable as a sum of losses over independent subsets of the data. This means conventional greedy, divide-and-conquer tree-building strategies do not apply. ROOT addresses this through a randomization-based tree construction with an explore-exploit strategy.

How ROOT works

The algorithm proceeds in several stages:

1. **Feature importance estimation:** Split probabilities are estimated using Ridge regression, Gradient Boosting Machine (GBM), or a user-supplied function, biasing the search toward covariates likely to be informative.

2. **Stochastic tree construction:** `num_trees` trees are grown. At each internal node, a feature is drawn according to the estimated split probabilities (or a "leaf" token is drawn, terminating the branch). Splits are made at the midpoint of the selected feature's empirical distribution. An explore-exploit strategy assigns leaf weights: with probability `explore_proba` a random weight is chosen; otherwise the greedy optimal weight (reducing the global objective) is used.
3. **Rashomon set selection:** Trees are ranked by their global objective values. The top-`k` trees (or all trees below a cutoff) form the Rashomon set: a collection of near-optimal but potentially different models, each providing a characterization of the optimal weight function.
4. **Aggregation:** Per-observation votes from the Rashomon set are combined (by default, majority vote) to produce the final weight vector `w_opt`.
5. **Characteristic tree:** A single summary decision tree is fitted to the aggregated `w_opt` assignments, providing a concise, interpretable description of the weight function.

Generalizability mode

When `generalizability_path = TRUE`, ROOT implements the methodology of Parikh et al. (2025) for characterizing underrepresented subgroups in trial-to-target generalizability analyses. In this mode:

- data must contain columns `Y` (outcome), `Tr` (treatment, 0/1), and `S` (sample indicator, 1 = trial, 0 = target).
- ROOT internally computes transportability scores based on inverse-probability weighting (IPW), estimates the selection model $P(S = 1 \mid X)$, and constructs Horvitz-Thompson-style influence scores.
- The default objective minimizes the variance of the weighted target average treatment effect (WTATE) estimator. This objective accounts for both the selection odds (trial participation probability) and treatment effect heterogeneity, so that subgroups are flagged as underrepresented only when they both lack trial representation and exhibit effect modification.
- The output includes the unweighted sample average treatment effect (SATE) and the WTATE with standard errors.

See [characterizing_underrep](#) for a higher-level wrapper that additionally produces a leaf-level summary table, and `vignette("generalizability_path_example")` for a worked example.

General optimization mode

When `generalizability_path = FALSE`, ROOT operates as a general functional optimizer. The user supplies any `data.frame` and (optionally) a custom `global_objective_fn`. If no objective is supplied, ROOT uses a default variance-based loss operating on the `vsq` column (per-unit variance proxy). See `vignette("optimization_path_example")` for an example.

References

Parikh H, Ross RK, Stuart E, Rudolph KE (2025). "Who Are We Missing?: A Principled Approach to Characterizing the Underrepresented Population." *Journal of the American Statistical Association*. doi:10.1080/01621459.2025.2495319

See Also

[characterizing_underrep](#) for a higher-level wrapper with leaf-summary output; `vignette("generalizability_path_example")` for the generalizability workflow; `vignette("optimization_path_example")` for general optimization.

Examples

```
## Not run:
# --- Generalizability mode ---
data(diabetes_data, package = "ROOT")
root_fit <- ROOT(
  data = diabetes_data,
  generalizability_path = TRUE,
  num_trees = 20,
  top_k_trees = TRUE,
  k = 10,
  seed = 123
)
summary(root_fit)
plot(root_fit)

# --- General optimization mode (custom objective) ---
my_objective <- function(D) {
  w <- D$w
  if (sum(w) == 0) return(Inf)
  sqrt(sum(w * D$vsq) / sum(w)^2)
}
opt_fit <- ROOT(
  data = my_data,
  global_objective_fn = my_objective,
  num_trees = 20,
  seed = 42
)

## End(Not run)
```

summary.characterizing_underrep

Summarize a characterizing_underrep fit

Description

Summarizes the ROOT summary which includes unweighted and (when in generalization mode) weighted estimates with standard errors, as reported by `summary.ROOT()`. Provides a brief overview of terminal rules from the annotated summary tree when available.

Usage

```
## S3 method for class 'characterizing_underrep'
summary(object, ...)
```

Arguments

<code>object</code>	A <code>characterizing_underrep</code> S3 object. Expected components include <code>root</code> which is a <code>ROOT</code> object (summarized by <code>summary.ROOT()</code>) and may contain <code>f</code> which is an <code>rpart</code> object for the summary tree, and <code>leaf_summary</code> which is a <code>data.frame</code> with one row per terminal node and may include a <code>rule</code> column of type <code>character</code> .
<code>...</code>	Currently unused. Included for S3 compatibility.

Details

Delegates core statistics and estimands to `summary(object$root)`. Previews up to ten terminal rules when a summary tree exists.

Value

object returned invisibly. Printed output is a readable summary.

Abbreviations

ATE Average treatment effect.

RCT Randomized controlled trial.

SE Standard error.

TATE Transported average treatment effect.

WTATE Weighted transported average treatment effect.

SATE Sample average treatment effect.

Examples

```
## Not run:
char.output = characterizing_underrep(diabetes_data, generalizability_path = TRUE, seed = 123)
summary(char.output)

## End(Not run)
```

summary.ROOT

Summarize a ROOT fit

Description

Provides a readable summary of a ROOT object, including:

1. the summary characterization tree `f`,
2. whether the user supplied a custom `global_objective_fn` (Yes/No), and
3. in generalizability mode (`generalizability_path = TRUE`), the unweighted and weighted estimands with their standard errors.

Usage

```
## S3 method for class 'ROOT'
summary(object, ...)
```

Arguments

<code>object</code>	A "ROOT" S3 object returned by <code>ROOT()</code> .
<code>...</code>	Currently unused and included for S3 compatibility.

Value

object returned invisibly. Printed output is for inspection.

Abbreviations

ATE Average treatment effect.

RCT Randomized controlled trial.

SE Standard error.

TATE Transported average treatment effect.

WTATE Weighted transported average treatment effect.

SATE Sample average treatment effect.

When `generalizability_path = TRUE`, the unweighted estimand corresponds to a SATE-type quantity and the weighted estimand to a WTATE-type quantity for the transported target population. When `generalizability_path = FALSE`, ROOT is used for general functional optimization and no causal labels are imposed; the summary focuses on the tree and diagnostics.

Diagnostics

The summary also reports:

- the number of trees grown,
- the size of the Rashomon set,
- the percentage of observations with ensemble vote `w_opt == 1`.

Examples

```
## Not run:  
ROOT.output = ROOT(diabetes_data, generalizability_path = TRUE, seed = 123)  
summary(ROOT.output)  
  
## End(Not run)
```

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