

# Package ‘caretEnsemble’

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**Type** Package

**Title** Ensembles of Caret Models

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<https://github.com/zachmayer/caretEnsemble>

**BugReports** <https://github.com/zachmayer/caretEnsemble/issues>

**Description** Functions for creating ensembles of caret models: caretList() and caretStack(). caretList() is a convenience function for fitting multiple caret::train() models to the same dataset. caretStack() will make linear or non-linear combinations of these models, using a caret::train() model as a meta-model.

**Depends** R (>= 4.1.0)

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---

as.caretList	<i>Convert object to caretList object</i>
--------------	---

---

**Description**

Converts object into a caretList

**Usage**

```
as.caretList(object)
```

**Arguments**

object	R Object
--------	----------

**Value**

a `caretList` object

---

as.caretList.default	<i>Convert object to caretList object - For Future Use</i>
----------------------	--

---

**Description**

Converts object into a caretList - For Future Use

**Usage**

```
## Default S3 method:  
as.caretList(object)
```

**Arguments**

object	R object
--------	----------

**Value**

NA

---

<code>as.caretList.list</code>	<i>Convert list to caretList</i>
--------------------------------	----------------------------------

---

**Description**

Converts list to caretList

**Usage**

```
## S3 method for class 'list'
as.caretList(object)
```

**Arguments**

<code>object</code>	list of caret models
---------------------	----------------------

**Value**

a `caretList` object

---

<code>autoplot.caretStack</code>	<i>Convenience function for more in-depth diagnostic plots of caretStack objects</i>
----------------------------------	--

---

**Description**

This function provides a more robust series of diagnostic plots for a `caretEnsemble` object.

**Usage**

```
## S3 method for class 'caretStack'
autoplot(object, training_data = NULL, xvars = NULL, show_class_id = 2L, ...)
```

**Arguments**

<code>object</code>	a <code>caretStack</code> object
<code>training_data</code>	The data used to train the ensemble. Required if <code>xvars</code> is not <code>NULL</code> Must be in the same row order as when the models were trained.
<code>xvars</code>	a vector of the names of x variables to plot against residuals
<code>show_class_id</code>	For classification only: which class level to show on the plot
<code>...</code>	ignored

**Value**

A grid of diagnostic plots. Top left is the range of the performance metric across each component model along with its standard deviation. Top right is the residuals from the ensembled model plotted against fitted values. Middle left is a bar graph of the weights of the component models. Middle right is the disagreement in the residuals of the component models (unweighted) across the fitted values. Bottom left and bottom right are the plots of the residuals against two random or user specified variables. Note that the ensemble must have been trained with `savePredictions = "final"`, which is required to get residuals from the stack for the plot.

**Examples**

```
set.seed(42)
data(models.reg)
ens <- caretStack(models.reg)
autoplot(ens)
```

---

c.caretList

*S3 definition for concatenating caretList*


---

**Description**

take N objects of class `caretList` and concatenate them into a larger object of class `caretList` for future ensembling

**Usage**

```
## S3 method for class 'caretList'
c(...)
```

**Arguments**

... the objects of class `caretList` or `train` to bind into a `caretList`

**Value**

a `caretList` object

**Examples**

```
data(iris)
model_list1 <- caretList(Sepal.Width ~ .,
  data = iris,
  tuneList = list(
    lm = caretModelSpec(method = "lm")
  )
)
model_list2 <- caretList(Sepal.Width ~ .,
```

```
data = iris, tuneLength = 1L,  
tuneList = list(  
  rf = caretModelSpec(method = "rf")  
)  
)  
  
bigList <- c(model_list1, model_list2)
```

---

c.train

*S3 definition for concatenating train objects*

---

## Description

take N objects of class train and concatenate into an object of class caretList for future ensembling

## Usage

```
## S3 method for class 'train'  
c(...)
```

## Arguments

... the objects of class train to bind into a caretList

## Value

a [caretList](#) object

## Examples

```
data(iris)  
model_lm <- caret::train(Sepal.Length ~ .,  
  data = iris,  
  method = "lm"  
)  
  
model_rf <- caret::train(Sepal.Length ~ .,  
  data = iris,  
  method = "rf",  
  tuneLength = 1L  
)  
  
model_list <- c(model_lm, model_rf)
```

---

caretEnsemble	<i>Combine several predictive models via weights</i>
---------------	--

---

### Description

Find a greedy, positive only linear combination of several `train` objects

Functions for creating ensembles of caret models: `caretList` and `caretStack`

### Usage

```
caretEnsemble(all.models, excluded_class_id = 0L, tuneLength = 1L, ...)
```

### Arguments

<code>all.models</code>	an object of class <code>caretList</code>
<code>excluded_class_id</code>	The integer level to exclude from binary classification or multiclass problems. By default no classes are excluded, as the greedy optimizer requires all classes because it cannot use negative coefficients.
<code>tuneLength</code>	The size of the grid to search for tuning the model. Defaults to 1, as the only parameter to optimize is the number of iterations, and the default of 100 works well.
<code>...</code>	additional arguments to pass <code>caret::train</code>

### Details

`greedyMSE` works well when you want an ensemble that will never be worse than any single model in the dataset. In the worst case scenario, it will select the single best model, if none of them can be ensembled to improve the overall score. It will also never assign any model a negative coefficient, which can help avoid unintuitive cases at prediction time (e.g. if the correlations between predictors breaks down on new data, negative coefficients can lead to bad results).

### Value

a `caretEnsemble` object

### Note

Every model in the "library" must be a separate `train` object. For example, if you wish to combine a random forests with several different values of `mtry`, you must build a model for each value of `mtry`. If you use several values of `mtry` in one `train` model, (e.g. `tuneGrid = expand.grid(.mtry=2:5)`), `caret` will select the best value of `mtry` before we get a chance to include it in the ensemble. By default, RMSE is used to ensemble regression models, and AUC is used to ensemble Classification models. This function does not currently support multi-class problems

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**See Also**

Useful links:

- <http://zachmayer.github.io/caretEnsemble/>
- <https://github.com/zachmayer/caretEnsemble>
- Report bugs at <https://github.com/zachmayer/caretEnsemble/issues>

**Examples**

```
set.seed(42)
models <- caretList(iris[1:50, 1:2], iris[1:50, 3], methodList = c("rpart", "rf"))
ens <- caretEnsemble(models)
summary(ens)
```

---

caretList

*Create a list of several train models from the caret package*

---

**Description**

Build a list of train objects suitable for ensembling using the [caretStack](#) function.

**Usage**

```
caretList(
  ...,
  trControl = NULL,
  methodList = NULL,
  tuneList = NULL,
  metric = NULL,
  continue_on_fail = FALSE,
  trim = TRUE
)
```



**Arguments**

...	arguments to pass to <code>train</code> . Don't use the formula interface, its slower and buggier compared to the X, y interface. Use a <code>data.table</code> for X. Particularly if you have a large dataset and/or many models, using a <code>data.table</code> will avoid unnecessary copies of your data and can save a lot of time and RAM. These arguments will determine which train method gets dispatched.
<code>trControl</code>	a <code>trainControl</code> object. If NULL, will use <code>defaultControl</code> .
<code>methodList</code>	optional, a character vector of caret models to ensemble. One of <code>methodList</code> or <code>tuneList</code> must be specified.
<code>tuneList</code>	optional, a NAMED list of <code>caretModelSpec</code> objects. This much more flexible than <code>methodList</code> and allows the specification of model-specific parameters (e.g. passing <code>trace=FALSE</code> to <code>nnet</code> )
<code>metric</code>	a string, the metric to optimize for. If NULL, we will choose a good one.
<code>continue_on_fail</code>	logical, should a valid <code>caretList</code> be returned that excludes models that fail, default is FALSE
<code>trim</code>	logical should the train models be trimmed to save memory and speed up stacking

**Value**

A list of `train` objects. If the model fails to build, it is dropped from the list.

**Examples**

```
caretList(
  Sepal.Length ~ Sepal.Width,
  head(iris, 50),
  methodList = c("glm", "lm"),
  tuneList = list(
    nnet = caretModelSpec(method = "nnet", trace = FALSE, tuneLength = 1)
  )
)
```

---

caretModelSpec

*Generate a specification for fitting a caret model*

---

**Description**

A caret model specification consists of 2 parts: a model (as a string) and the arguments to the train call for fitting that model

**Usage**

```
caretModelSpec(method = "rf", ...)
```

**Arguments**

method	the modeling method to pass to caret::train
...	Other arguments that will eventually be passed to caret::train

**Value**

a list of lists

**Examples**

```
caretModelSpec("rf", tuneLength = 5, preProcess = "ica")
```

---

caretStack	<i>Combine several predictive models via stacking</i>
------------	---

---

**Description**

Stack several [train](#) models using a [train](#) model.

**Usage**

```
caretStack(
  all.models,
  new_X = NULL,
  new_y = NULL,
  metric = NULL,
  trControl = NULL,
  excluded_class_id = 1L,
  ...
)
```

**Arguments**

all.models	a caretList, or an object coercible to a caretList (such as a list of train objects)
new_X	Data to predict on for the caretList, prior to training the stack (for transfer learning). if NULL, the stacked predictions will be extracted from the caretList models.
new_y	The outcome variable to predict on for the caretList, prior to training the stack (for transfer learning). If NULL, will use the observed levels from the first model in the caret stack. If 0, will include all levels.
metric	the metric to use for grid search on the stacking model.
trControl	a trainControl object to use for training the ensemble model. If NULL, will use defaultControl.
excluded_class_id	The integer level to exclude from binary classification or multiclass problems.
...	additional arguments to pass to the stacking model

## Details

Uses either transfer learning or stacking to stack models. Assumes that all models were trained on the same number of rows of data, with the same target values. The features, cross-validation strategies, and model types (class vs reg) may vary however. If your stack of models were trained with different number of rows, please provide `new_X` and `new_y` so the models can predict on a common set of data for stacking.

If your models were trained on different columns, you should use stacking.

If you have both differing rows and columns in your model set, you are out of luck. You need at least a common set of rows during training (for stacking) or a common set of columns at inference time for transfer learning.

## Value

S3 `caretStack` object

## References

Caruana, R., Niculescu-Mizil, A., Crew, G., & Ksikes, A. (2004). Ensemble Selection from Libraries of Models. <https://www.cs.cornell.edu/~caruana/ctp/ct.papers/caruana.icml04.icdm06long.pdf>

## Examples

```
models <- caretList(  
  x = iris[1:50, 1:2],  
  y = iris[1:50, 3],  
  methodList = c("rpart", "glm")  
)  
caretStack(models, method = "glm")
```

---

defaultControl

*Construct a default train control for use with caretList*

---

## Description

Unlike `caret::trainControl`, this function defaults to 5 fold CV. CV is good for stacking, as every observation is in the test set exactly once. We use 5 instead of 10 to save compute time, as `caretList` is for fitting many models. We also construct explicit fold indexes and return the stacked predictions, which are needed for stacking. For classification models we return class probabilities.

## Usage

```
defaultControl(  
  target,  
  method = "cv",  
  number = 5L,  
  savePredictions = "final",
```

```

index = caret::createFolds(target, k = number, list = TRUE, returnTrain = TRUE),
is_class = is.factor(target) || is.character(target),
is_binary = length(unique(target)) == 2L,
...
)

```

### Arguments

target	the target variable.
method	the method to use for trainControl.
number	the number of folds to use.
savePredictions	the type of predictions to save.
index	the fold indexes to use.
is_class	logical, is this a classification or regression problem.
is_binary	logical, is this binary classification.
...	other arguments to pass to <a href="#">trainControl</a>

---

defaultMetric	<i>Construct a default metric</i>
---------------	-----------------------------------

---

### Description

Caret defaults to RMSE for classification and RMSE for regression. For classification, I would rather use ROC.

### Usage

```
defaultMetric(is_class, is_binary)
```

### Arguments

is_class	logical, is this a classification or regression problem.
is_binary	logical, is this binary classification.

---

dotplot.caretStack      *Comparison dotplot for a caretStack object*

---

### Description

This is a function to make a dotplot from a caretStack. It uses dotplot from the caret package on all the models in the ensemble, excluding the final ensemble model. At the moment, this function only works if the ensembling model has the same number of resamples as the component models.

### Usage

```
## S3 method for class 'caretStack'
dotplot(x, ...)
```

### Arguments

x                      An object of class caretStack  
 ...                    passed to dotplot

### Examples

```
set.seed(42)
models <- caretList(
  x = iris[1:100, 1:2],
  y = iris[1:100, 3],
  methodList = c("rpart", "glm")
)
meta_model <- caretStack(models, method = "lm")
lattice::dotplot(meta_model)
```

---

extractMetric              *Generic function to extract accuracy metrics from various model objects*

---

### Description

A generic function to extract cross-validated accuracy metrics from model objects.

### Usage

```
extractMetric(x, ...)
```

### Arguments

x                      An object from which to extract metrics. The specific method will be dispatched based on the class of x.  
 ...                    Additional arguments passed to the specific methods.

**Value**

A `data.table`

**See Also**

`extractMetric.train`, `extractMetric.caretList`, `extractMetric.caretStack`

---

`extractMetric.caretList`

*Extract accuracy metrics from a `caretList` object*

---

**Description**

Extract the cross-validated accuracy metrics from each model in a `caretList`.

**Usage**

```
## S3 method for class 'caretList'  
extractMetric(x, ...)
```

**Arguments**

<code>x</code>	a <code>caretList</code> object
<code>...</code>	passed to <code>extractMetric.train</code>

**Value**

A `data.table` with metrics from each model.

---

`extractMetric.caretStack`

*Extract accuracy metrics from a `caretStack` object*

---

**Description**

Extract the cross-validated accuracy metrics from the ensemble model and individual models in a `caretStack`.

**Usage**

```
## S3 method for class 'caretStack'  
extractMetric(x, ...)
```

**Arguments**

x                    a caretStack object  
 ...                  passed to extractMetric.train and extractMetric.caretList

**Value**

A data.table with metrics from the ensemble model and individual models.

---

extractMetric.train    *Extract accuracy metrics from a [train](#) model*

---

**Description**

Extract the cross-validated accuracy metrics and their SDs from caret.

**Usage**

```
## S3 method for class 'train'
extractMetric(x, metric = NULL, ...)
```

**Arguments**

x                    a train object  
 metric              a character string representing the metric to extract.  
 ...                  ignored If NULL, uses the metric that was used to train the model.

**Value**

A numeric representing the metric desired metric.

---

greedyMSE              *Greedy optimization for MSE*

---

**Description**

Greedy optimization for minimizing the mean squared error. Works for classification and regression.

**Usage**

```
greedyMSE(X, Y, max_iter = 100L)
```

**Arguments**

X	A numeric matrix of features.
Y	A numeric matrix of target values.
max_iter	An integer scalar of the maximum number of iterations.

**Value**

A list with components:

model_weights	A numeric matrix of model_weights.
RMSE	A numeric scalar of the root mean squared error.
max_iter	An integer scalar of the maximum number of iterations.

---

greedyMSE_caret	<i>caret interface for greedyMSE</i>
-----------------	--------------------------------------

---

**Description**

caret interface for greedyMSE. greedyMSE works well when you want an ensemble that will never be worse than any single predictor in the dataset. It does not use an intercept and it does not allow for negative coefficients. This makes it highly constrained and in general does not work well on standard classification and regression problems. However, it does work well in the case of: \* The predictors are highly correlated with each other \* The predictors are highly correlated with the model \* You expect or want positive only coefficients In the worse case, this method will select one input and use that, but in many other cases it will return a positive, weighted average of the inputs. Since it never uses negative weights, you never get into a scenario where one model is weighted negative and on new data you get were predictions because a correlation changed. Since this model will always be a positive weighted average of the inputs, it will rarely do worse than the individual models on new data.

**Usage**

```
greedyMSE_caret()
```



---

 permutationImportance *Permutation Importance*


---

### Description

Permute each variable in a dataset and use the change in predictions to calculate the importance of each variable. Based on the scikit learn implementation of permutation importance: [https://scikit-learn.org/stable/modules/permutation\\_importance.html](https://scikit-learn.org/stable/modules/permutation_importance.html). However, we don't compare to the target by a metric. We JUST look at the change in the model's predictions, as measured by MAE. (for classification, this is like using a Brier score). We shuffle each variable and recompute the predictions before and after the shuffle. The difference in MAE. is the importance of that variable. We normalize by computing the MAE of the shuffled original predictions as an upper bound on the MAE and divide by this value. So a variable that, when shuffled, caused predictions as bad as shuffling the output predictions, we know that variable is 100. Similarly, as with regular permutation importance, a variable that, when shuffled, gives the same MAE as the original model has an importance of 0.

This method cannot yield negative importances. It is merely a measure of how much the models uses the variable, and does not tell you which variables help or hurt generalization. Use the model's cross-validated metrics to assess generalization.

### Usage

```
permutationImportance(model, newdata, normalize = TRUE)
```

### Arguments

model	A train object from the caret package.
newdata	A data.frame of new data to use to compute importances. Can be the training data.
normalize	A logical indicating whether to normalize the importances to sum to one.

### Value

A named numeric vector of variable importances.

---

 plot.caretList *Plot a caretList object*


---

### Description

This function plots the performance of each model in a caretList object.

### Usage

```
## S3 method for class 'caretList'
plot(x, metric = NULL, ...)
```

**Arguments**

x	a caretList object
metric	which metric to plot
...	ignored

**Value**

A ggplot2 object

---

plot.caretStack	<i>Plot a caretStack object</i>
-----------------	---------------------------------

---

**Description**

This function plots the performance of each model in a caretList object.

**Usage**

```
## S3 method for class 'caretStack'
plot(x, metric = NULL, ...)
```

**Arguments**

x	a caretStack object
metric	which metric to plot. If NULL, will use the default metric used to train the model.
...	ignored

**Value**

a ggplot2 object

---

predict.caretList	<i>Create a matrix of predictions for each of the models in a caretList</i>
-------------------	---

---

**Description**

Make a matrix of predictions from a list of caret models

**Usage**

```
## S3 method for class 'caretList'
predict(object, newdata = NULL, verbose = FALSE, excluded_class_id = 1L, ...)
```

**Arguments**

object	an object of class caretList
newdata	New data for predictions. It can be NULL, but this is ill-advised.
verbose	Logical. If FALSE no progress bar is printed if TRUE a progress bar is shown. Default FALSE.
excluded_class_id	Integer. The class id to drop when predicting for multiclass
...	Other arguments to pass to <code>predict.train</code>

---

predict.caretStack      *Make predictions from a caretStack*

---

**Description**

Make predictions from a caretStack. This function passes the data to each function in turn to make a matrix of predictions, and then multiplies that matrix by the vector of weights to get a single, combined vector of predictions.

**Usage**

```
## S3 method for class 'caretStack'
predict(
  object,
  newdata = NULL,
  se = FALSE,
  level = 0.95,
  excluded_class_id = 0L,
  return_class_only = FALSE,
  verbose = FALSE,
  ...
)
```

**Arguments**

object	a <code>caretStack</code> to make predictions from.
newdata	a new dataframe to make predictions on
se	logical, should prediction errors be produced? Default is false.
level	tolerance/confidence level should be returned
excluded_class_id	Which class to exclude from predictions. Note that if the caretStack was trained with an excluded_class_id, that class is ALWAYS excluded from the predictions from the caretList of input models. excluded_class_id for predict.caretStack is for the final ensemble model. So different classes could be excluded from the caretList models and the final ensemble model.

return_class_only	a logical indicating whether to return only the class predictions as a factor. If TRUE, the return will be a factor rather than a data.table. This is a convenience function, and should not be widely used. For example if you have a downstream process that consumes the output of the model, you should have that process consume probabilities for each class. This will make it easier to change prediction probability thresholds if needed in the future.
verbose	a logical indicating whether to print progress
...	arguments to pass to <code>predict.train</code> for the ensemble model. Do not specify type here. For classification, type will always be prob, and for regression, type will always be raw.

### Details

Prediction weights are defined as variable importance in the stacked caret model. This is not available for all cases such as where the library model predictions are transformed before being passed to the stacking model.

### Value

a data.table of predictions

### Examples

```
models <- caretList(
  x = iris[1:100, 1:2],
  y = iris[1:100, 3],
  methodList = c("rpart", "glm")
)
meta_model <- caretStack(models, method = "lm")
RMSE(predict(meta_model, iris[101:150, 1:2]), iris[101:150, 3])
```

---

predict.greedyMSE      *Predict method for greedyMSE*

---

### Description

Predict method for greedyMSE objects.

### Usage

```
## S3 method for class 'greedyMSE'
predict(object, newdata, return_labels = FALSE, ...)
```

**Arguments**

object            A greedyMSE object.  
newdata           A numeric matrix of new data.  
return\_labels    A logical scalar of whether to return labels.  
...               Additional arguments. Ignored.

**Value**

A numeric matrix of predictions.

---

`print.caretStack`        *Print a caretStack object*

---

**Description**

This is a function to print a caretStack.

**Usage**

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

**Arguments**

x                 An object of class caretStack  
...               ignored

**Examples**

```
models <- caretList(  
  x = iris[1:100, 1:2],  
  y = iris[1:100, 3],  
  methodList = c("rpart", "glm")  
)  
meta_model <- caretStack(models, method = "lm")  
print(meta_model)
```

---

print.greedyMSE	<i>Print method for greedyMSE</i>
-----------------	-----------------------------------

---

**Description**

Print method for greedyMSE objects.

**Usage**

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

**Arguments**

x	A greedyMSE object.
...	Additional arguments. Ignored.

---

print.summary.caretList	<i>Print a summary.caretList object</i>
-------------------------	---

---

**Description**

This is a function to print a summary.caretList

**Usage**

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

**Arguments**

x	An object of class summary.caretList
...	ignored

---

```
print.summary.caretStack
```

*Print a summary.caretStack object*

---

### Description

This is a function to print a summary.caretStack.

### Usage

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

### Arguments

x	An object of class summary.caretStack
...	ignored

---

```
summary.caretList
```

*Summarize a caretList*

---

### Description

This function summarizes the performance of each model in a caretList object.

### Usage

```
## S3 method for class 'caretList'  
summary(object, metric = NULL, ...)
```

### Arguments

object	a caretList object
metric	The metric to show. If NULL will use the metric used to train each model
...	passed to extractMetric

### Value

A data.table with metrics from each model.

summary.caretStack      *Summarize a caretStack object*

---

### Description

This is a function to summarize a caretStack.

### Usage

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

### Arguments

object	An object of class caretStack
...	ignored

### Examples

```
models <- caretList(  
  x = iris[1:100, 1:2],  
  y = iris[1:100, 3],  
  methodList = c("rpart", "glm")  
)  
meta_model <- caretStack(models, method = "lm")  
summary(meta_model)
```

---

tuneCheck      *Check that the tuning parameters list supplied by the user is valid*

---

### Description

This function makes sure the tuning parameters passed by the user are valid and have the proper naming, etc.

### Usage

```
tuneCheck(x)
```

### Arguments

x	a list of user-supplied tuning parameters and methods
---	---



---

varImp.caretStack	<i>Variable importance for caretStack</i>
-------------------	---

---

**Description**

This is a function to extract variable importance from a caretStack.

**Usage**

```
## S3 method for class 'caretStack'
varImp(object, newdata = NULL, normalize = TRUE, ...)
```

**Arguments**

object	An object of class caretStack
newdata	the data to use for computing importance. If NULL, will use the stacked predictions from the models.
normalize	a logical indicating whether to normalize the importances to sum to one.
...	passed to predict.caretList

---

varImp.greedyMSE	<i>variable importance for a greedyMSE model</i>
------------------	--

---

**Description**

Variable importance for a greedyMSE model.

**Usage**

```
## S3 method for class 'greedyMSE'
varImp(object, ...)
```

**Arguments**

object	A greedyMSE object.
...	Additional arguments. Ignored.

---

wtd.sd	<i>Calculate a weighted standard deviation</i>
--------	--

---

**Description**

Used to weight deviations among ensembled model predictions

**Usage**

```
wtd.sd(x, w, na.rm = FALSE)
```

**Arguments**

x	a numeric vector
w	a vector of weights equal to length of x
na.rm	a logical indicating how to handle missing values, default = TRUE

---

[.caretList	<i>Index a caretList</i>
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---

**Description**

Index a caret list to extract caret models into a new caretList object

**Usage**

```
## S3 method for class 'caretList'  
object[index]
```

**Arguments**

object	an object of class caretList
index	selected index

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