

Package ‘ICEbox’

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Author Alex Goldstein, Adam Kapelner, Justin Bleich

Maintainer Adam Kapelner <kapelner@qc.cuny.edu>

Description Implements Individual Conditional Expectation (ICE) plots, a tool for visualizing the model estimated by any supervised learning algorithm. ICE plots refine Friedman's partial dependence plot by graphing the functional relationship between the predicted response and a covariate of interest for individual observations. Specifically, ICE plots highlight the variation in the fitted values across the range of a covariate of interest, suggesting where and to what extent they may exist.

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Depends sfsmisc

Suggests randomForest, MASS

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clusterICE

Clustering of ICE and d-ICE curves by kmeans.

Description

Clustering of ICE and d-ICE curves by kmeans. All curves are centered to have mean 0 and then kmeans is applied to the curves with the specified number of clusters.

Usage

```
clusterICE(ice_obj, nClusters, plot = TRUE, plot_margin = 0.05,
           colorvec, plot_pdp = FALSE, x_quantile = FALSE,
           avg_lwd = 3, centered = FALSE,
           plot_legend = FALSE, ...)
```

Arguments

ice_obj	Object of class ice or dice to cluster.
nClusters	Number of clusters to find.
plot	If TRUE, plots the clusters.
plot_margin	Extra margin to pass to ylim as a fraction of the range of cluster centers.
colorvec	Optional vector of colors to use for each cluster.
plot_pdp	If TRUE, the PDP (ice object) or d-PDP (dice object) is plotted with a dotted black line and highlighted in yellow.
x_quantile	If TRUE, the plot is drawn with the x-axis taken to be quantile(gridpts). If FALSE, the predictor's original scale is used.
avg_lwd	Average line width to use when plotting the cluster means. Line width is proportional to the cluster's size.
centered	If TRUE, all cluster means are shifted to be to be 0 at the minimum value of the predictor. If FALSE, the original cluster means are used.
plot_legend	If TRUE a legend mapping line colors to the proportion of the data in each cluster is added to the plot.
...	Additional arguments for plotting.

Value

The output of the kmeans call (a list of class kmeans).

See Also

ice, dice

Examples

```
## Not run:
require(ICEbox)
require(randomForest)
require(MASS) #has Boston Housing data, Pima

data(Boston) #Boston Housing data
X = Boston
y = X$medv
X$medv = NULL

## build a RF:
bh_rf = randomForest(X, y)

## Create an 'ice' object for the predictor "age":
bh.ice = ice(object = bh_rf, X = X, y = y, predictor = "age",
            frac_to_build = .1)

## cluster the curves into 2 groups.
clusterICE(bh.ice, nClusters = 2, plot_legend = TRUE)

## cluster the curves into 3 groups, start all at 0.
clusterICE(bh.ice, nClusters = 3, plot_legend = TRUE, center = TRUE)

## End(Not run)
```

dice *Creates an object of class dice.*

Description

Estimates the partial derivative function for each curve in an ice object. See Goldstein et al (2013) for further details.

Usage

```
dice(ice_obj, DerivEstimator)
```

Arguments

ice_obj Object of class `ice`. This function generates partial derivative estimates for each row in `ice_obj$ice_curves`.

DerivEstimator Optional function with a single argument `y`. Returns the estimated partial derivative of a function sampled at the points `(ice_obj$gridpts,y)`. If omitted, the default (a) smooths `(ice_obj$gridpts,y)` using `supsmu` and then (b) uses the `D1tr` function ("discrete first derivative using simple difference ratios") found in the `sfsmisc` package to estimate the derivative.

Value

A list of class `dice` with the following elements. Most are passed directly through from `ice_object` and exist to enable various plotting facilities.

<code>d_ice_curves</code>	Matrix of dimension <code>nrow(Xice)</code> by <code>length(gridpts)</code> . Each row corresponds to an observation's d-ICE curve, estimated at the values of predictor in <code>gridpts</code> .
<code>xj</code>	The actual values of predictor observed in the data in the order of <code>Xice</code> .
<code>actual_deriv</code>	Vector of length <code>nrow(Xice)</code> containing the estimated partial derivatives at the value of the predictor actually found in <code>Xice</code> .
<code>sd_deriv</code>	Vector of length <code>length(gridpts)</code> with the cross-observation sd of partial derivative estimates. For instance <code>sd_deriv[1]</code> equals <code>sd(d_ice_curves[,1])</code> .
<code>logodds</code>	Passed from <code>ice_object</code> . If TRUE, <code>d_ice_curves</code> are estimated derivatives of the centered log-odds.
<code>gridpts</code>	Passed from <code>ice_object</code> .
<code>predictor</code>	Passed from <code>ice_object</code> .
<code>xlab</code>	Passed from <code>ice_object</code> .
<code>nominal_axis</code>	Passed from <code>ice_object</code> .
<code>range_y</code>	Passed from <code>ice_object</code> .
<code>Xice</code>	Passed from <code>ice_object</code> .
<code>dmdp</code>	The estimated partial derivative of the PDP.

References

Goldstein, A., Kapelner, A., Bleich, J., and Pitkin, E., Peeking Inside the Black Box: Visualizing Statistical Learning With Plots of Individual Conditional Expectation. (2014) *Journal of Computational and Graphical Statistics*, in press

Martin Maechler et al. `sfsmisc`: Utilities from Seminar fuer Statistik ETH Zurich. R package version 1.0-24.

See Also

`plot.dice`, `print.dice`, `summary.dice`

Examples

```
## Not run:
# same examples as for 'ice', but now create a derivative estimate as well.
require(ICEbox)
require(randomForest)
require(MASS) #has Boston Housing data, Pima

##### regression example
data(Boston) #Boston Housing data
X = Boston
y = X$medv
```

```

X$medv = NULL

## build a RF:
bhd_rf_mod = randomForest(X, y)

## Create an 'ice' object for the predictor "age":
bhd.ice = ice(object = bhd_rf_mod, X = X, y = y, predictor = "age", frac_to_build = .1)

# make a dice object:
bhd.dice = dice(bhd.ice)

#### classification example
data(Pima.te) #Pima Indians diabetes classification
y = Pima.te$type
X = Pima.te
X$type = NULL

## build a RF:
pima_rf = randomForest(x = X, y = y)

## Create an 'ice' object for the predictor "skin":
# For classification we plot the centered log-odds. If we pass a predict
# function that returns fitted probabilities, setting logodds = TRUE instructs
# the function to set each ice curve to the centered log-odds of the fitted
# probability.
pima.ice = ice(object = pima_rf, X = X, predictor = "skin", logodds = TRUE,
              predictfcn = function(object, newdata){
                predict(object, newdata, type = "prob")[, 2]
              }
            )

# make a dice object:
pima.dice = dice(pima.ice)

## End(Not run)

```

ice

Creates an object of class ice.

Description

Creates an ice object with individual conditional expectation curves for the passed model object, X matrix, predictor, and response. See Goldstein et al (2013) for further details.

Usage

```
ice(object, X, y, predictor, predictfcn, verbose = TRUE, frac_to_build = 1,
    indices_to_build = NULL, num_grid_pts, logodds = FALSE, probit = FALSE, ...)
```

Arguments

<code>object</code>	The fitted model to estimate ICE curves for.
<code>X</code>	The design matrix we wish to estimate ICE curves for. Rows are observations, columns are predictors. Typically this is taken to be <code>object</code> 's training data, but this is not strictly necessary.
<code>y</code>	Optional vector of the response values <code>object</code> was trained on. It is used to compute y-axis ranges that are useful for plotting. If not passed, the range of predicted values is used and a warning is printed.
<code>predictor</code>	The column number or variable name in <code>X</code> of the predictor of interest, ($x_S = X[,j]$).
<code>predictfcn</code>	Optional function that accepts two arguments, <code>object</code> and <code>newdata</code> , and returns an N vector of <code>object</code> 's predicted response for data <code>newdata</code> . If this argument is not passed, the procedure attempts to find a generic <code>predict</code> function corresponding to <code>class(object)</code> .
<code>verbose</code>	If TRUE, prints messages about the procedure's progress.
<code>frac_to_build</code>	Number between 0 and 1, with 1 as default. For large <code>X</code> matrices or fitted models that are slow to make predictions, specifying <code>frac_to_build</code> less than 1 will choose a subset of the observations to build curves for. The subset is chosen such that the remaining observations' values of <code>predictor</code> are evenly spaced throughout the quantiles of the full <code>X[,predictor]</code> vector.
<code>indices_to_build</code>	Vector of indices, $\subset \{1, \dots, \text{row}(X)\}$ specifying which observations to build ICE curves for. As this is an alternative to setting <code>frac_to_build</code> , both cannot be specified.
<code>num_grid_pts</code>	Optional number of values in the range of <code>predictor</code> at which to estimate each curve. If missing, the curves are estimated at each unique value of <code>predictor</code> in the <code>X</code> observations we estimate ICE curves for.
<code>logodds</code>	If TRUE, for classification creates PDPs by plotting the centered log-odds implied by the fitted probabilities. We assume that the generic or passed <code>predict</code> function returns probabilities, and so the flag tells us to transform these to centered logits after the predictions are generated. Note: <code>probit</code> cannot be TRUE.
<code>probit</code>	If TRUE, for classification creates PDPs by plotting the probit implied by the fitted probabilities. We assume that the generic or passed <code>predict</code> function returns probabilities, and so the flag tells us to transform these to probits after the predictions are generated. Note: <code>logodds</code> cannot be TRUE.
<code>...</code>	Other arguments to be passed to <code>object</code> 's generic <code>predict</code> function.

Value

A list of class `ice` with the following elements.

<code>gridpts</code>	Sorted values of <code>predictor</code> at which each curve is estimated. Duplicates are removed – by definition, elements of <code>gridpts</code> are unique.
<code>ice_curves</code>	Matrix of dimension <code>nrow(X)</code> by <code>length(gridpts)</code> . Each row corresponds to an observation's ICE curve, estimated at the values of <code>predictor</code> in <code>gridpts</code> .

<code>xj</code>	The actual values of predictor observed in the data in the order of <code>Xice</code> .
<code>actual_predictions</code>	Vector of length <code>nrow(X)</code> containing the model's predictions at the actual value of the predictors in the order of <code>Xice</code> .
<code>xlab</code>	String with the predictor name corresponding to <code>predictor</code> . If <code>predictor</code> is a column number, <code>xlab</code> is set to <code>colnames(X)[, predictor]</code> .
<code>nominal_axis</code>	If TRUE, <code>length(gridpts)</code> is 5 or fewer; otherwise FALSE. When TRUE the plot function treats the x-axis as if <code>x</code> is nominal.
<code>range_y</code>	If <code>y</code> was passed, the range of the response. Otherwise it defaults to be <code>max(ice_curves) - min(ice_curves)</code> and a message is printed to the console.
<code>sd_y</code>	If <code>y</code> was passed, the standard deviation of the response. Otherwise it is defaults to <code>sd(actual_predictions)</code> and a message is printed to the console.
<code>Xice</code>	A matrix containing the subset of <code>X</code> for which ICE curves are estimated. Observations are ordered to be increasing in predictor. This ordering is the same one as in <code>ice_curves</code> , <code>xj</code> and <code>actual_predictions</code> , meaning for all these objects the <code>i</code> -th element refers to the same observation in <code>X</code> .
<code>pdp</code>	A vector of size <code>length(gridpts)</code> which is a numerical approximation to the partial dependence function (PDP) corresponding to the estimated ICE curves. See Goldstein et al (2013) for a discussion of how the PDP is a form of post-processing. See Friedman (2001) for a description of PDPs.
<code>predictor</code>	Same as the argument, see argument description.
<code>logodds</code>	Same as the argument, see argument description.
<code>indices_to_build</code>	Same as the argument, see argument description.
<code>frac_to_build</code>	Same as the argument, see argument description.
<code>predictfcn</code>	Same as the argument, see argument description.

References

- Jerome Friedman. Greedy Function Approximation: A Gradient Boosting Machine. *The Annals of Statistics*, 29(5): 1189-1232, 2001.
- Goldstein, A., Kapelner, A., Bleich, J., and Pitkin, E., Peeking Inside the Black Box: Visualizing Statistical Learning With Plots of Individual Conditional Expectation. (2014) *Journal of Computational and Graphical Statistics*, in press

See Also

`plot.ice`, `print.ice`, `summary.ice`

Examples

```
## Not run:
require(ICEbox)
require(randomForest)
require(MASS) #has Boston Housing data, Pima
```

```
##### regression example
data(Boston) #Boston Housing data
X = Boston
y = X$medv
X$medv = NULL

## build a RF:
bhd_rf_mod = randomForest(X, y)

## Create an 'ice' object for the predictor "age":
bhd.ice = ice(object = bhd_rf_mod, X = X, y = y, predictor = "age", frac_to_build = .1)

#### classification example
data(Pima.te) #Pima Indians diabetes classification
y = Pima.te$type
X = Pima.te
X$type = NULL

## build a RF:
pima_rf_mod = randomForest(x = X, y = y)

## Create an 'ice' object for the predictor "skin":
# For classification we plot the centered log-odds. If we pass a predict
# function that returns fitted probabilities, setting logodds = TRUE instructs
# the function to set each ice curve to the centered log-odds of the fitted
# probability.
pima.ice = ice(object = pima_rf_mod, X = X, predictor = "skin", logodds = TRUE,
              predictfcn = function(object, newdata){
                predict(object, newdata, type = "prob")[, 2]
              }
              )

## End(Not run)
```

plot.dice

Create a plot of a dice object.

Description

Plotting of dice objects.

Usage

```
## S3 method for class 'dice'
plot(x, plot_margin = 0.05, frac_to_plot = 1,
     plot_sd = TRUE, plot_orig_pts_deriv = TRUE, pts_preds_size = 1.5,
     colorvec, color_by = NULL, x_quantile = TRUE, plot_dpdp = TRUE,
     rug_quantile = seq(from = 0, to = 1, by = 0.1), ...)
```


Arguments

x	Object of class dice to plot.
plot_margin	Extra margin to pass to ylim as a fraction of the range of x\$d_ice_curves.
frac_to_plot	If frac_to_plot is less than 1, randomly plot frac_to_plot fraction of the curves in x\$d_ice_curves.
plot_sd	If TRUE, plot the cross-observation sd of partial derivatives below the derivative plots.
plot_orig_pts_deriv	If TRUE, marks each curve at the location of the derivative estimate at the location of predictor actually occurring in the data. If FALSE no mark is drawn.
pts_preds_size	Size of points to make if plot_orig_pts_deriv is TRUE.
colorvec	Optional vector of colors to use for each curve.
color_by	Optional variable name (or column number) in Xice to color curves by. If the color_by variable has 10 or fewer unique values, a discrete set of colors is used for each value and a legend is printed and returned. If there are more values, curves are colored from light to dark corresponding to low to high values of the variable specified by color_by.
x_quantile	If TRUE, the plot is drawn with the x-axis taken to be quantile(gridpts). If FALSE, the predictor's original scale is used.
plot_dpdp	If TRUE, the estimated derivative of the PDP is plotted and highlighted in yellow.
rug_quantile	If not null, tick marks are drawn on the x-axis corresponding to the vector of quantiles specified by this parameter. Forced to NULL when x_quantile is set to TRUE.
...	Additional plotting arguments.

Value

A list with the following elements.

plot_points_indices	Row numbers of Xice of those observations presented in the plot.
legend_text	If the color_by argument was used, a legend describing the map between the color_by predictor and curve colors.

See Also

dice

Examples

```
## Not run:
require(ICEbox)
require(randomForest)
require(MASS) #has Boston Housing data, Pima

data(Boston) #Boston Housing data
```

```

X = Boston
y = X$medv
X$medv = NULL

## build a RF:
bhd_rf_mod = randomForest(X, y)

## Create an 'ice' object for the predictor "age":
bhd.ice = ice(object = bhd_rf_mod, X = X, y = y, predictor = "age", frac_to_build = .1)

# estimate derivatives, then plot.
bhd.dice = dice(bhd.ice)
plot(bhd.dice)

## End(Not run)

```

plot.ice

Plotting of ice objects.

Description

Plotting of ice objects.

Usage

```

## S3 method for class 'ice'
plot(x, plot_margin = 0.05, frac_to_plot = 1,
     plot_points_indices = NULL, plot_orig_pts_preds = TRUE,
     pts_preds_size = 1.5, colorvec, color_by = NULL,
     x_quantile = TRUE, plot_pdp = TRUE,
     centered = FALSE, prop_range_y = TRUE,
     rug_quantile = seq(from = 0, to = 1, by = 0.1),
     centered_percentile = 0,
     point_labels = NULL, point_labels_size = NULL,
     prop_type,...)

```

Arguments

x	Object of class ice to plot.
plot_margin	Extra margin to pass to ylim as a fraction of the range of x\$ice_curves.
frac_to_plot	If frac_to_plot is less than 1, randomly plot frac_to_plot fraction of the curves in x\$ice_curves.
plot_points_indices	If not NULL, this plots only the indices of interest. If not NULL, frac_to_plot must be 1 otherwise an error is thrown. Default is NULL.
plot_orig_pts_preds	If TRUE, marks each curve at the location of the observation's actual fitted value. If FALSE, no mark is drawn.

pts_preds_size	Size of points to make if plot_origin_pts_preds is TRUE.
colorvec	Optional vector of colors to use for each curve.
color_by	Optional variable name in Xice, column number in Xice, or data vector of the correct length to color curves by. If the color_by variable has 10 or fewer unique values, a discrete set of colors is used for each value and a legend is printed and returned. If there are more values, curves are colored from light to dark corresponding to low to high values of the variable specified by color_by.
x_quantile	If TRUE, the plot is drawn with the x-axis taken to be quantile(gridpts). If FALSE, the predictor's original scale is used.
plot_pdp	If TRUE, the PDP is plotted and highlighted in yellow.
centered	If TRUE, all curves are re-centered to be 0 at the quantile given by centered_percentile. See Goldstein et al (2013) for details and examples. If FALSE, the original ice_curves are plotted.
prop_range_y	When TRUE and centered=TRUE as well, the range of the right vertical axis displays the centered values as a fraction of the sd of the fitted values on actual observations if prop_type is missing or set to "sd". If prop_type is set to "range", the right axis displays the centered values as a fraction of the range of the fitted values over the actual observations.
centered_percentile	The percentile of predictor for which all ice_curves are "pinched together" and set to be 0. Default is .01.
point_labels	If not NULL, labels to plot next to each point. Default is NULL.
point_labels_size	If not NULL, size of labels to plot next to each point. Default is NULL which means it's the size of pts_preds_size.
rug_quantile	If not NULL, tick marks are drawn on the x-axis corresponding to the vector of quantiles specified by this parameter. Forced to NULL when x_quantile is set to TRUE.
prop_type	Scaling factor for the right vertical axis in centered plots if prop_range_y is TRUE. Can be one of "sd" (default) or "range". Ignored if centered and prop_range_y are not both TRUE.
...	Other arguments to be passed to the plot function.

Value

A list with the following elements.

plot_points_indices	Row numbers of Xice of those observations presented in the plot.
legend_text	If the color_by argument was used, a legend describing the map between the color_by predictor and curve colors.

See Also

ice

Examples

```

## Not run:
require(ICEbox)
require(randomForest)
require(MASS) #has Boston Housing data, Pima

data(Boston) #Boston Housing data
X = Boston
y = X$medv
X$medv = NULL

## build a RF:
bhd_rf_mod = randomForest(X, y)

## Create an 'ice' object for the predictor "age":
bhd.ice = ice(object = bhd_rf_mod, X = X, y = y, predictor = "age",
             frac_to_build = .1)

## plot
plot(bhd.ice, x_quantile = TRUE, plot_pdp = TRUE, frac_to_plot = 1)

## centered plot
plot(bhd.ice, x_quantile = TRUE, plot_pdp = TRUE, frac_to_plot = 1,
     centered = TRUE)

## color the curves by high and low values of 'rm'.
# First create an indicator variable which is 1 if the number of
# rooms is greater than the median:
median_rm = median(X$rm)
bhd.ice$I_rm = ifelse(bhd.ice$rm > median_rm, 1, 0)

plot(bhd.ice, frac_to_plot = 1, centered = TRUE, prop_range_y = TRUE,
     x_quantile = T, plot_orig_pts_preds = T, color_by = "I_rm")
bhd.ice = ice(object = bhd_rf_mod, X = X, y = y, predictor = "age",
             frac_to_build = 1)
plot(bhd.ice, frac_to_plot = 1, centered = TRUE, prop_range_y = TRUE,
     x_quantile = T, plot_orig_pts_preds = T, color_by = y)

## End(Not run)

```

print.dice

Print method for dice objects.

Description

Prints a summary of a dice object.

Usage

```

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

```

Arguments

x	Object of class dice.
...	Ignored for now.

print.ice	<i>Print method for ice objects.</i>
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Description

Prints a summary of an ice object.

Usage

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

Arguments

x	Object of class ice.
...	Ignored for now.

summary.dice	<i>Summary function for dice objects.</i>
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Description

Alias of print method.

Usage

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

Arguments

object	Object of class dice.
...	Ignored for now.

summary.ice	<i>Summary function for ice objects.</i>
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Description

Alias of print method.

Usage

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

Arguments

object	Object of class ice.
...	Ignored for now.

WhiteWine	<i>Data concerning white wine.</i>
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Description

The WhiteWine data frame has 4898 rows and 12 columns and concerns white wines from a region in Portugal. The response variable, quality, is a wine quality metric, taken to be the median preference score of three blind tasters on a scale of 1-10. The 11 covariates are physicochemical metrics of wine quality such as citric acid content, sulphates, etc.

Usage

```
data(WhiteWine)
```

Format

A data frame of 4898 cases on 12 variables.

Source

K Bache and M Lichman. UCI machine learning repository, 2013. <http://archive.ics.uci.edu/ml>

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