SHAP Documentation

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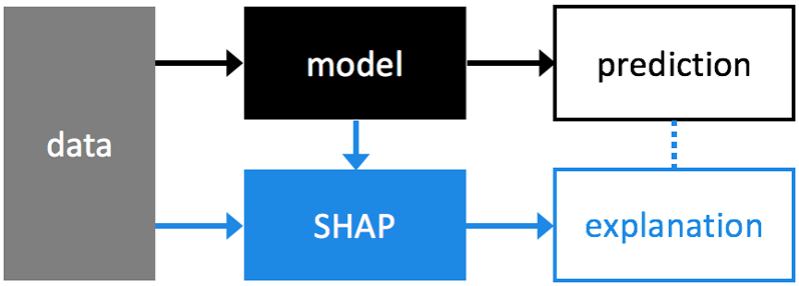

SHAP (SHapley Additive exPlanations) is a unified approach to explain the output of any machine learning model. SHAP connects game theory with local explanations, uniting several previous methods and representing the only possible consistent and locally accurate additive feature attribution method based on expectations (see the SHAP NIPS paper for details).

class shap.**TreeExplainer**(*model*, *data=None*, *model_output='margin'*, *feature_dependence='tree_path_dependent'*)

Uses Tree SHAP algorithms to explain the output of ensemble tree models.

Tree SHAP is a fast and exact method to estimate SHAP values for tree models and ensembles of trees, under several different possible assumptions about feature dependence. It depends on fast C++ implementations either inside an externel model package or in the local compiled C extention.

model [model object] The tree based machine learning model that we want to explain. XGBoost, LightGBM, CatBoost, and most tree-based scikit-learn models are supported.

data [numpy.array or pandas.DataFrame] The background dataset to use for integrating out features. This argument is optional when feature_dependence="tree_path_dependent", since in that case we can use the number of training samples that went down each tree path as our background dataset (this is recorded in the model object).

feature_dependence ["tree_path_dependent" (default) or "independent"] Since SHAP values rely on conditional expectations we need to decide how to handle correlated (or otherwise dependent) input features. The default "tree_path_dependent" approach is to just follow the trees and use the number of training examples that went down each leaf to represent the background distribution. This approach repects feature dependecies along paths in the trees. However, for non-linear marginal transforms (like explaining the model loss) we don't yet have fast algorithms that respect the tree path dependence, so instead we offer an "independent" approach that breaks the dependencies between features, but allows us to explain non-linear transforms of the model's output. Note that the "independent" option requires a background dataset and its runtime scales linearly with the size of the background dataset you use. Anywhere from 100 to 1000 random background samples are good sizes to use.

model_output ["margin", "probability", or "log_loss"] What output of the model should be explained. If "margin" then we explain the raw output of the trees, which varies by model (for binary classification in XGBoost this is the log odds ratio). If "probability" then we explain the output of the model transformed into probability space (note that this means the SHAP values now sum to the probability output of the model). If "log_loss" then we explain the log base e of the model loss function, so that the SHAP values sum up to the log loss of the model for each sample. This is helpful for breaking down model performance by feature. Currently the probability and log_loss options are only supported when feature_dependence="independent".

shap_interaction_values(*X*, *y=None*, *tree_limit=None*)

Estimate the SHAP interaction values for a set of samples.

X [numpy.array, pandas.DataFrame or catboost.Pool (for catboost)] A matrix of samples (# samples x # features) on which to explain the model's output.

y [numpy.array] An array of label values for each sample. Used when explaining loss functions (not yet supported).

tree_limit [None (default) or int] Limit the number of trees used by the model. By default None means no use the limit of the original model, and -1 means no limit.

For models with a single output this returns a tensor of SHAP values (# samples x # features x # features). The matrix (# features x # features) for each sample sums to the difference between the model output for that sample and the expected value of the model output (which is stored in the expected_value attribute of the explainer). Each row of this matrix sums to the SHAP value for that feature for that sample. The diagonal entries of the matrix represent the "main effect" of that feature on the prediction and the symmetric off-diagonal entries represent the interaction effects between all pairs of features for that sample. For models with vector outputs this returns a list of tensors, one for each output.

shap_values(*X*, *y=None*, *tree_limit=None*, *approximate=False*)

Estimate the SHAP values for a set of samples.

X [numpy.array, pandas.DataFrame or catboost.Pool (for catboost)] A matrix of samples (# samples x # features) on which to explain the model's output.

y [numpy.array] An array of label values for each sample. Used when explaining loss functions.

tree_limit [None (default) or int] Limit the number of trees used by the model. By default None means no use the limit of the original model, and -1 means no limit.

approximate [bool] Run fast, but only roughly approximate the Tree SHAP values. This runs a method previously proposed by Saabas which only considers a single feature ordering. Take care since this does not have the consistency guarantees of Shapley values and places too much weight on lower splits in the tree.

For models with a single output this returns a matrix of SHAP values (# samples x # features). Each row sums to the difference between the model output for that sample and the expected value of the model output (which is stored in the expected_value attribute of the explainer when it is constant). For models with vector outputs this returns a list of such matrices, one for each output.

class shap.**KernelExplainer**(*model*, *data*, *link=<shap.common.IdentityLink object>*, ***kwargs*)

Uses the Kernel SHAP method to explain the output of any function.

Kernel SHAP is a method that uses a special weighted linear regression to compute the importance of each feature. The computed importance values are Shapley values from game theory and also coefficents from a local linear regression.

model [function or iml.Model] User supplied function that takes a matrix of samples (# samples x # features) and computes a the output of the model for those samples. The output can be a vector (# samples) or a matrix (# samples x # model outputs).

data [numpy.array or pandas.DataFrame or shap.common.DenseData or any scipy.sparse matrix] The background dataset to use for integrating out features. To determine the impact of a feature, that feature is set to "missing" and the change in the model output is observed. Since most models aren't designed to handle arbitrary missing data at test time, we simulate "missing" by replacing the feature with the values it takes in the background dataset. So if the background dataset is a simple sample of all zeros, then we would approximate a feature being missing by setting it to zero. For small problems this background dataset can be the whole training set, but for larger problems consider using a single reference value or using the kmeans function to summarize the dataset. Note: for sparse case we accept any sparse matrix but convert to lil format for performance.

link ["identity" or "logit"] A generalized linear model link to connect the feature importance values to the model output. Since the feature importance values, phi, sum up to the model output, it often makes sense to connect them to the ouput with a link function where link(outout) = sum(phi). If the model output is a probability then the LogitLink link function makes the feature importance values have log-odds units.

shap_values(*X*, ***kwargs*)

Estimate the SHAP values for a set of samples.

X [numpy.array or pandas.DataFrame or any scipy.sparse matrix] A matrix of samples (# samples x # features) on which to explain the model's output.

nsamples ["auto" or int] Number of times to re-evaluate the model when explaining each prediction. More samples lead to lower variance estimates of the SHAP values. The "auto" setting uses *nsamples = 2 * X.shape[1] + 2048*.

l1_reg ["num_features(int)", "auto" (default for now, but deprecated), "aic", "bic", or float] The l1 regularization to use for feature selection (the estimation procedure is based on a debiased lasso). The auto option currently uses "aic" when less that 20% of the possible sample space is enumerated, otherwise it uses no regularization. THE BEHAVIOR OF "auto" WILL CHANGE in a future version to be based on num_features instead of AIC. The "aic" and "bic" options use the AIC and BIC rules for regularization. Using "num_features(int)" selects a fix number of top features. Passing a float directly sets the "alpha" parameter of the sklearn.linear_model.Lasso model used for feature selection.

For models with a single output this returns a matrix of SHAP values (# samples x # features). Each row sums to the difference between the model output for that sample and the expected value of the model output (which is stored as expected_value attribute of the explainer). For models with vector outputs this returns a list of such matrices, one for each output.

class shap.**DeepExplainer**(*model*, *data*, *session=None*, *learning_phase_flags=None*)

Meant to approximate SHAP values for deep learning models.

This is an enhanced version of the DeepLIFT algorithm (Deep SHAP) where, similar to Kernel SHAP, we approximate the conditional expectations of SHAP values using a selection of background samples. Lundberg and Lee, NIPS 2017 showed that the per node attribution rules in DeepLIFT (Shrikumar, Greenside, and Kundaje, arXiv 2017) can be chosen to approximate Shapley values. By integrating over many backgound samples DeepExplainer estimates approximate SHAP values such that they sum up to the difference between the expected model output on the passed background samples and the current model output (f(x) - E[f(x)]).

shap_values(*X*, *ranked_outputs=None*, *output_rank_order='max'*)

Return approximate SHAP values for the model applied to the data given by X.

X [list,] if framework == 'tensorflow': numpy.array, or pandas.DataFrame if framework == 'pytorch': torch.tensor A tensor (or list of tensors) of samples (where X.shape[0] == # samples) on which to explain the model's output.

ranked_outputs [None or int] If ranked_outputs is None then we explain all the outputs in a multi-output model. If ranked_outputs is a positive integer then we only explain that many of the top model outputs (where "top" is determined by output_rank_order). Note that this causes a pair of values to be returned (shap_values, indexes), where shap_values is a list of numpy arrays for each of the output ranks, and indexes is a matrix that indicates for each sample which output indexes were choses as "top".

output_rank_order ["max", "min", or "max_abs"] How to order the model outputs when using ranked_outputs, either by maximum, minimum, or maximum absolute value.

For a models with a single output this returns a tensor of SHAP values with the same shape as X. For a model with multiple outputs this returns a list of SHAP value tensors, each of which are the same shape as X. If ranked_outputs is None then this list of tensors matches the number of model outputs. If ranked_outputs is a positive integer a pair is returned (shap_values, indexes), where shap_values is a list of tensors with a length of ranked_outputs, and indexes is a matrix that indicates for each sample which output indexes were chosen as "top".

CHAPTER 1

Plots

shap.**summary_plot**(*shap_values*, *features=None*, *feature_names=None*, *max_display=None*, *plot_type='dot'*, *color=None*, *axis_color='#333333'*, *title=None*, *alpha=1*, *show=True*, *sort=True*, *color_bar=True*, *auto_size_plot=True*, *layered_violin_max_num_bins=20*, *class_names=None*)

Create a SHAP summary plot, colored by feature values when they are provided.

shap_values [numpy.array] Matrix of SHAP values (# samples x # features)

features [numpy.array or pandas.DataFrame or list] Matrix of feature values (# samples x # features) or a feature_names list as shorthand

feature_names [list] Names of the features (length # features)

max_display [int] How many top features to include in the plot (default is 20, or 7 for interaction plots)

plot_type ["dot" (default) or "violin"] What type of summary plot to produce

shap.**dependence_plot**(*ind*, *shap_values*, *features*, *feature_names=None*, *display_features=None*, *interaction_index='auto'*, *color='#1E88E5'*, *axis_color='#333333'*, *dot_size=16*, *x_jitter=0*, *alpha=1*, *title=None*, *xmin=None*, *xmax=None*, *show=True*)

Create a SHAP dependence plot, colored by an interaction feature.

Plots the value of the feature on the x-axis and the SHAP value of the same feature on the y-axis. This shows how the model depends on the given feature, and is like a richer extenstion of the classical parital dependence plots. Vertical dispersion of the data points represents interaction effects. Grey ticks along the y-axis are data points where the feature's value was NaN.

ind [int or string] If this is an int it is the index of the feature to plot. If this is a string it is either the name of the feature to plot, or it can have the form "rank(int)" to specify the feature with that rank (ordered by mean absolute SHAP value over all the samples).

shap_values [numpy.array] Matrix of SHAP values (# samples x # features).

features [numpy.array or pandas.DataFrame] Matrix of feature values (# samples x # features).

feature_names [list] Names of the features (length # features).

display_features [numpy.array or pandas.DataFrame] Matrix of feature values for visual display (such as strings instead of coded values).

interaction_index ["auto", None, int, or string] The index of the feature used to color the plot. The name of a feature can also be passed as a string. If "auto" then shap.common.approximate_interactions is used to pick what seems to be the strongest interaction (note that to find to true stongest interaction you need to compute the SHAP interaction values).

x_jitter [float (0 - 1)] Adds random jitter to feature values. May increase plot readability when feature is discrete.

alpha [float] The transparency of the data points (between 0 and 1). This can be useful to the show density of the data points when using a large dataset.

xmin [float or string] Represents the lower bound of the plot's x-axis. It can be a string of the format "percentile(float)" to denote that percentile of the feature's value used on the x-axis.

xmax [float or string] Represents the upper bound of the plot's x-axis. It can be a string of the format "percentile(float)" to denote that percentile of the feature's value used on the x-axis.

shap.**force_plot**(*base_value*, *shap_values*, *features=None*, *feature_names=None*, *out_names=None*, *link='identity'*, *plot_cmap='RdBu'*, *matplotlib=False*, *show=True*, *figsize=(20, 3)*, *ordering_keys=None*, *ordering_keys_time_format=None*)

Visualize the given SHAP values with an additive force layout.

shap.**image_plot**(*shap_values*, *x*, *labels=None*, *show=True*)

Plots SHAP values for image inputs.

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