## **Exploring Learner Predictions**

Learners use features to learn a prediction function and make predictions, but the effect of those features is often not apparent. mlr (http://www.rdocumentation.org/packages/mlr/) can estimate the partial dependence of a learned function on a subset of the feature space using generatePartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html).

Partial dependence plots reduce the potentially high dimensional function estimated by the learner, and display a marginalized version of this function in a lower dimensional space. For example suppose  $Y=f(X)+\epsilon$  where  $\mathbb{E}[\epsilon|X]=0$  With (X,Y) pairs drawn independently from this statistical model, a learner may estimate  $\hat{f}$ , which, if X is high dimensional, can be uninterpretable. Suppose we want to approximate the relationship between some subset of X. We partition X into two sets,  $X_s$  and  $X_c$  such that  $X=X_s\cup X_c$  where  $X_s$  is a subset of X of interest.

The partial dependence of f on  $X_s$  is

$$f_{X_s} = \mathbb{E}_{X_c} f(X_s, X_c).$$

 $X_c$  is integrated out. We use the following estimator:

$$\hat{f}_{\left|X_{s}
ight|}=rac{1}{N}\sum_{i=1}^{N}\hat{f}\left(X_{s},x_{ic}
ight).$$

The individual conditional expectation of an observation can also be estimated using the above algorithm absent the averaging, giving  $\hat{f}_{X_s}^{(i)}$ . This allows the discovery of features of  $\hat{f}$  that may be obscured by an aggregated summary of  $\hat{f}$ .

The partial derivative of the partial dependence function,  $\frac{\partial \hat{f}_{X_s}}{\partial X_s}$ , and the individual conditional expectation function,  $\frac{\partial \hat{f}_{X_s}}{\partial X_s}$ , can also be computed. For regression and survival tasks the partial derivative of a single feature  $X_s$  is the gradient of the partial dependence function, and for classification tasks where the learner can output class probabilities the Jacobian. Note that if the learner produces discontinuous partial dependence (e.g., piecewise constant functions such as decision trees, ensembles of decision trees, etc.) the derivative will be 0 (where the function is not changing) or trending towards positive or negative infinity (at the discontinuities where the derivative is undefined). Plotting the partial dependence function of such learners may give the impression that the function is not discontinuous because the prediction grid is not composed of all discontinuous points in the predictor space. This results in a line interpolating that makes the function appear to be piecewise linear (where the derivative would be defined except at the boundaries of each piece).

The partial derivative can be informative regarding the additivity of the learned function in certain features. If  $\hat{f}_{X_s}^{(i)}$  is an additive function in a feature  $X_s$ , then its partial derivative will not depend on any other features ( $X_c$ ) that may have been used by the learner. Variation in the estimated partial derivative indicates that there is a region of interaction between  $X_s$  and  $X_c$  in  $\hat{f}$ . Similarly, instead of using the mean to estimate the expected value of the function at different values of  $X_s$ , instead computing the variance can highlight regions of interaction between  $X_s$  and  $X_c$ .

See Goldstein, Kapelner, Bleich, and Pitkin (2014) (http://arxiv.org/abs/1309.6392) for more details and their package ICEbox (http://www.rdocumentation.org/packages/ICEbox/) for the original implementation. The algorithm works for any supervised learner with classification, regression, and survival tasks.

## Generating partial dependences

Our implementation, following mlr (http://www.rdocumentation.org/packages/mlr/)'s visualization (../visualization/index.html) pattern, consists of the above mentioned function generatePartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html), as well as two visualization functions, plotPartialDependence (http://www.rdocumentation.org/packages/mlr/functions/plotPartialDependence.html) and plotPartialDependenceGGVIS (http://www.rdocumentation.org/packages/mlr/functions/plotPartialDependenceGGVIS.html). The former generates input (objects of class PartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/PartialDependenceData.html)) for the latter.

The first step executed by generatePartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html) is to generate a feature grid for every element of the character vector features passed. The data are given by the input argument, which can be a Task (http://www.rdocumentation.org/packages/mlr/functions/Task.html) or a data.frame (http://www.rdocumentation.org/packages/base/functions/data.frame.html). The feature grid can be generated in several ways. A uniformly spaced grid of length gridsize (default 10) from the empirical minimum to the empirical maximum is created by default, but arguments fmin and fmax may be used to override the empirical default (the lengths of fmin and fmax must match the length of features). Alternatively the feature data can be resampled, either by using a bootstrap or by subsampling.

```
lrn.classif = makeLearner("classif.ksvm", predict.type = "prob")
fit.classif = train(lrn.classif, iris.task)
pd = generatePartialDependenceData(fit.classif, iris.task, "Petal.Width")
pd
#> PartialDependenceData
#> Task: iris-example
#> Features: Petal.Width
#> Target: setosa, versicolor, virginica
#> Derivative: FALSE
#> Interaction: FALSE
#> Individual: FALSE
   Class Probability Petal.Width
#> 1 setosa 0.4983925 0.1000000
            0.4441165 0.3666667
#> 3 setosa 0.3808075 0.6333333
#> 4 setosa 0.3250243 0.9000000
#> 5 setosa 0.2589014
                        1.1666667
#> 6 setosa 0.1870692 1.4333333
#> ... (30 rows, 3 cols)
```

As noted above,  $X_s$  does not have to be unidimensional. If it is not, the <code>interaction</code> flag must be set to <code>TRUE</code>. Then the individual feature grids are combined using the Cartesian product, and the estimator above is applied, producing the partial dependence for every combination of unique feature values. If the <code>interaction</code> flag is <code>FALSE</code> (the default) then by default  $X_s$  is assumed unidimensional, and partial dependencies are generated for each feature separately. The resulting output when <code>interaction = FALSE</code> has a column for each feature, and <code>NA</code> where the feature was not used.

```
pd.lst = generatePartialDependenceData(fit.classif, iris.task, c("Petal.Width", "Petal.Length"), FALSE)
head(pd.lst$data)
   Class Probability Petal.Width Petal.Length
NA
#> 2 setosa 0.4441165 0.3666667
NA
                                       NA
#> 5 setosa 0.2589014 1.1666667
#> 6 setosa 0.1870692 1.4333333
                                       MA
tail(pd.lst$data)
      Class Probability Petal.Width Petal.Length
#> 55 virginica 0.2006336 NA 3.622222
#> 56 virginica 0.3114545
                               NA 4.277778
#> 57 virginica 0.4404613
                              NA 4.933333
#> 58 virginica 0.6005358 NA 5.588889
#> 59 virginica 0.7099841 NA 6.244444
#> 60 virginica 0.7242584 NA 6.900000
```

```
pd.int = generatePartialDependenceData(fit.classif, iris.task, c("Petal.Width", "Petal.Length"), TRUE)
pd.int
#> PartialDependenceData
#> Task: iris-example
#> Features: Petal.Width, Petal.Length
#> Target: setosa, versicolor, virginica
#> Derivative: FALSE
#> Interaction: TRUE
#> Individual: FALSE
   Class Probability Petal.Width Petal.Length
#> 1 setosa 0.6885025 0.1000000 1
            0.6824560 0.3666667
#> 3 setosa 0.6459476 0.6333333
#> 4 setosa 0.5750861 0.9000000
#> 5 setosa 0.4745925 1.1666667
#> 6 setosa 0.3749285 1.4333333
#> ... (300 rows, 4 cols)
```

At each step in the estimation of  $\hat{f}_{X_s}$  a set of predict.type = "prob" this entails the mean class probabilities. However, other summaries of the predictions may be used. For regression and survival tasks the function used here must either return one number or three, and, if the latter, the numbers must be sorted lowest to highest. For classification tasks the function must return a number for each level of the target feature.

As noted, the  $\lceil \text{fun} \rceil$  argument can be a function which returns three numbers (sorted low to high) for a regression task. This allows further exploration of relative feature importance. If a feature is relatively important, the bounds are necessarily tighter because the feature accounts for more of the variance of the predictions, i.e., it is "used" more by the learner. More directly setting  $\lceil \text{fun} \rceil = \text{var} \rceil$  identifies regions of interaction between  $X_s$  and  $X_c$ .

```
lrn.regr = makeLearner("regr.ksvm")
fit.regr = train(lrn.regr, bh.task)
pd.regr = generatePartialDependenceData(fit.regr, bh.task, "lstat", fun = median)
pd.regr
#> PartialDependenceData
#> Task: BostonHousing-example
#> Target: medv
#> Derivative: FALSE
#> Interaction: FALSE
#> Individual: FALSE
       medv
#> 1 24.69031 1.730000
#> 2 23.72479 5.756667
#> 3 22.34841 9.783333
#> 4 20.78817 13.810000
#> 5 19.76183 17.836667
#> 6 19.33115 21.863333
#> ... (10 rows, 2 cols)
```

```
pd.ci = generatePartialDependenceData(fit.regr, bh.task, "lstat",
 fun = function(x) quantile(x, c(.25, .5, .75)))
pd.ci
#> PartialDependenceData
#> Task: BostonHousing-example
#> Features: 1stat
#> Target: medv
#> Derivative: FALSE
#> Interaction: FALSE
#> Individual: FALSE
       medv lstat lower
                                   upper
#> 1 24.69031 1.730000 21.36068 29.75615
#> 2 23.72479 5.756667 20.80590 28.02338
#> 3 22.34841 9.783333 20.06507 25.22291
#> 4 20.78817 13.810000 18.55592 23.68100
#> 5 19.76183 17.836667 16.52737 22.98520
#> 6 19.33115 21.863333 15.14425 22.12766
#> ... (10 rows, 4 cols)
```

```
pd.classif = generatePartialDependenceData(fit.classif, iris.task, "Petal.Length", fun = median)
pd.classif
#> PartialDependenceData
#> Task: iris-example
#> Features: Petal.Length
#> Target: setosa, versicolor, virginica
#> Derivative: FALSE
#> Interaction: FALSE
#> Individual: FALSE
#> Class Probability Petal.Length
#> 1 setosa 0.31008788 1.000000
#> 2 setosa 0.24271454
                        1.655556
                        2.311111
#> 3 setosa 0.17126036
#> 4 setosa 0.09380787
#> 5 setosa 0.04579912 3.622222
#> 6 setosa 0.02455344
                         4.277778
#> ... (30 rows, 3 cols)
```

In addition to bounds based on a summary of the distribution of the conditional expectation of each observation, learners which can estimate the variance of their predictions can also be used. The argument bounds is a numeric vector of length two which is added (so the first number should be negative) to the point prediction to produce a confidence interval for the partial dependence. The default is the .025 and .975 quantiles of the Gaussian distribution.

```
fit.se = train(makeLearner("regr.randomForest", predict.type = "se"), bh.task)
pd.se = generatePartialDependenceData(fit.se, bh.task, c("lstat", "crim"))
head(pd.se$data)
       medv
                 lstat crim
                             lower
                                      upper
#> 1 31.02186 1.730000 NA 27.65357 34.39015
#> 2 25.94429 5.756667 NA 23.43079 28.45779
#> 3 23.52758 9.783333 NA 21.23661 25.81856
#> 4 22.05223 13.810000 NA 20.30446 23.80000
#> 5 20.44293 17.836667 NA 18.72603 22.15982
#> 6 19.80143 21.863333 NA 18.04932 21.55353
tail(pd.se$data)
        medv 1stat
                      crim lower
                                       upper
#> 15 21.65846 NA 39.54849 19.50827 23.80866
#> 16 21.64409 NA 49.43403 19.49704 23.79114
#> 17 21.63038 NA 59.31957 19.48054 23.78023
#> 18 21.61514
                NA 69.20512 19.46092 23.76936
#> 19 21.61969
                NA 79.09066 19.46819 23.77119
#> 20 21.61987 NA 88.97620 19.46843 23.77130
```

As previously mentioned if the aggregation function is not used, i.e., it is the identity, then the conditional expectation of  $\hat{f}_{X_s}^{(i)}$  is estimated. If individual = TRUE then generatePartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html) returns n partial dependence estimates made at each point in the prediction grid constructed from the features.

```
pd.ind.regr = generatePartialDependenceData(fit.regr, bh.task, "lstat", individual = TRUE)
pd.ind.regr
#> PartialDependenceData
#> Task: BostonHousing-example
#> Features: 1stat
#> Target: medv
#> Derivative: FALSE
#> Interaction: FALSE
#> Individual: TRUE
#> Predictions centered: FALSE
       medv lstat idx
#> 1 25.66995 1.730000 1
#> 2 24.71747 5.756667
#> 3 23.64157 9.783333
#> 4 22.70812 13.810000
#> 5 22.00059 17.836667
#> 6 21.46195 21.863333
#> ... (5060 rows, 3 cols)
```

The resulting output, particularly the element data in the returned object, has an additional column idx which gives the index of the observation to which the row pertains.

```
pd.ind.classif = generatePartialDependenceData(fit.classif, iris.task, "Petal.Length", individual = TRUE)
pd.ind.classif
#> PartialDependenceData
#> Task: iris-example
#> Features: Petal.Length
#> Target: setosa, versicolor, virginica
#> Derivative: FALSE
#> Interaction: FALSE
#> Individual: TRUE
#> Predictions centered: FALSE
    Class Probability Petal.Length
#> 1 setosa 0.9814053 1 1.setosa
                               1 2.setosa
#> 2 setosa 0.9747355
#> 3 setosa 0.9815516
                                1 3.setosa
#> 4 setosa 0.9795761
                                1 4.setosa
#> 5 setosa 0.9806494
                               1 5.setosa
#> 6 setosa 0.9758763
                               1 6.setosa
#> ... (4500 rows, 4 cols)
```

Individual estimates of partial dependence can also be centered by predictions made at all n observations for a particular point in the prediction grid created by the features. This is controlled by the argument center which is a list of the same length as the length of the features argument and contains the values of the features desired.

```
iris = getTaskData(iris.task)
pd.ind.classif = generatePartialDependenceData(fit.classif, iris.task, "Petal.Length", individual = TRUE,
    center = list("Petal.Length" = min(iris$Petal.Length)))
```

Partial derivatives can also be computed for individual partial dependence estimates and aggregate partial dependence. This is restricted to a single feature at a time. The derivatives of individual partial dependence estimates can be useful in finding regions of interaction between the feature for which the derivative is estimated and the features excluded.

```
pd.classif.der = generatePartialDependenceData(fit.classif, iris.task, "Petal.Width", derivative = TRUE)
head(pd.classif.der$data)

#> Class Probability Petal.Width
#> 1 setosa -0.1479385    0.1000000

#> 2 setosa -0.2422728    0.3666667

#> 3 setosa -0.2189893    0.6333333

#> 4 setosa -0.2162803    0.9000000

#> 5 setosa -0.2768042    1.1666667

#> 6 setosa -0.2394176    1.4333333
```

## **Functional ANOVA**

Hooker (2004) (http://dl.acm.org/citation.cfm?id=1014122) proposed the decomposition of a learned function  $\hat{f}$  as a sum of lower dimensional functions

$$f(\mathbf{x}) = g_0 + \sum_{i=1}^p g_i(X_i) + \sum_{i 
eq j} g_{ij}(x_{ij}) + \ldots$$

where p is the number of features. generateFunctionalANOVAData (http://www.rdocumentation.org/packages/mlr/functions/generateFunctionalANOVAData.html) estimates the individual g functions using partial dependence. When functions depend only on one feature, they are equivalent to partial dependence, but a g function which depends on more than one feature is the "effect" of only those features: lower dimensional "effects" are removed.

$$\hat{g}_{u}(X) = rac{1}{N} \sum_{i=1}^{N} \left( \hat{f}\left(X
ight) - \sum_{v \subset u} g_{v}(X) 
ight)$$

Here u is a subset of  $1, \ldots, p$ . When |v| = 1  $g_v$  can be directly computed by computing the bivariate partial dependence of  $\hat{f}$  on  $X_u$  and then subtracting off the univariate partial dependences of the features contained in v.

Although this decomposition is generalizable to classification it is currently only available for regression tasks.

```
lrn.regr = makeLearner("regr.ksvm")
fit.regr = train(lrn.regr, bh.task)
fa = generateFunctionalANOVAData(fit.regr, bh.task, "lstat", depth = 1, fun = median)
#> FunctionalANOVAData
#> Task: BostonHousing-example
#> Features: 1stat
#> Target: medv
#> effect medv
                       lstat
#> 1 1stat 24.89524 1.730000
#> 2 1stat 23.76025 5.756667
#> 3 1stat 22.35052 9.783333
#> 4 1stat 20.68435 13.810000
#> 5 1stat 19.60062 17.836667
#> 6 1stat 19.01178 21.863333
#> ... (10 rows, 3 cols)
pd.regr = generatePartialDependenceData(fit.regr, bh.task, "lstat", fun = median)
pd.regr
#> PartialDependenceData
#> Task: BostonHousing-example
#> Features: 1stat
#> Target: medv
#> Derivative: FALSE
#> Interaction: FALSE
#> Individual: FALSE
#>
    medv lstat
#> 1 24.89524 1.730000
#> 2 23.76025 5.756667
#> 3 22.35052 9.783333
#> 4 20.68435 13.810000
#> 5 19.60062 17.836667
#> 6 19.01178 21.863333
#> ... (10 rows, 2 cols)
```

The depth argument is similar to the interaction argument in generatePartialDependenceData

(http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html) but instead of specifying whether all of joint "effect" of all the features is computed, it determines whether "effects" of all subsets of the features given the specified depth are computed. So, for example, with p features and depth 1, the univariate partial dependence is returned. If, instead, depth 2, then all possible bivariate functional ANOVA effects are returned. This is done by computing the univariate partial dependence for each feature and subtracting it from the bivariate partial dependence for each possible pair.

```
fa.bv = generateFunctionalANOVAData(fit.regr, bh.task, c("crim", "lstat", "age"),
 depth = 2)
fa.bv
#> FunctionalANOVAData
#> Task: BostonHousing-example
#> Features: crim, lstat, age
#> Target: medv
#>
                   medv
       effect
                            crim 1stat age
#> 1 crim:lstat -22.68734 0.006320 1.73 NA
#> 2 crim:lstat -23.22114 9.891862 1.73 NA
#> 3 crim:1stat -24.77479 19.777404 1.73 NA
#> 4 crim:lstat -26.41395 29.662947 1.73 NA
#> 5 crim:lstat -27.56524 39.548489 1.73 NA
#> 6 crim:1stat -28.27952 49.434031 1.73 NA
#> ... (300 rows, 5 cols)
names(table(fa.bv$data$effect)) ## interaction effects estimated
#> [1] "crim:age" "crim:lstat" "lstat:age"
```

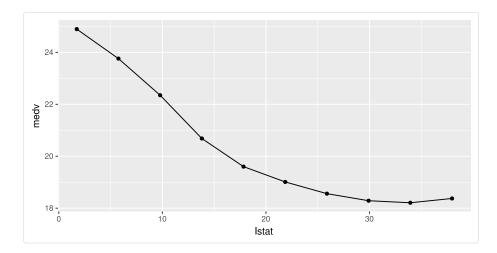
## Plotting partial dependences

Results from generatePartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html) and generateFunctionalANOVAData (http://www.rdocumentation.org/packages/mlr/functions/generateFunctionalANOVAData.html) can be visualized with plotPartialDependence (http://www.rdocumentation.org/packages/mlr/functions/plotPartialDependence.html) and plotPartialDependenceGGVIS

(http://www.rdocumentation.org/packages/mlr/functions/plotPartialDependenceGGVIS.html).

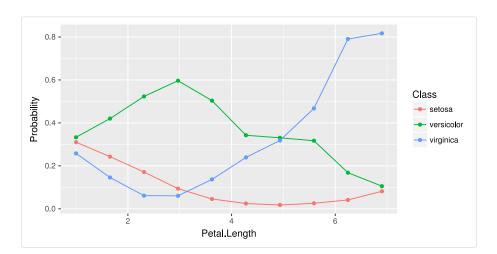
With one feature and a regression task the output is a line plot, with a point for each point in the corresponding feature's grid.

plotPartialDependence(pd.regr)



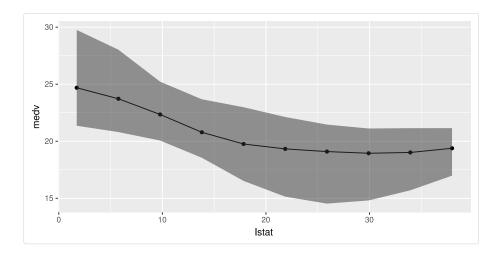
With a classification task, a line is drawn for each class, which gives the estimated partial probability of that class for a particular point in the feature grid.

plotPartialDependence(pd.classif)



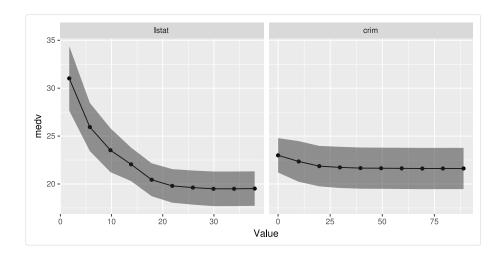
For regression tasks, when the fun argument of generatePartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html) is used, the bounds will automatically be displayed using a gray ribbon.

plotPartialDependence(pd.ci)



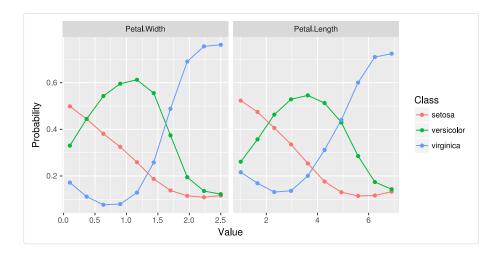
The same goes for plots of partial dependences where the learner has predict.type = "se".

plotPartialDependence(pd.se)



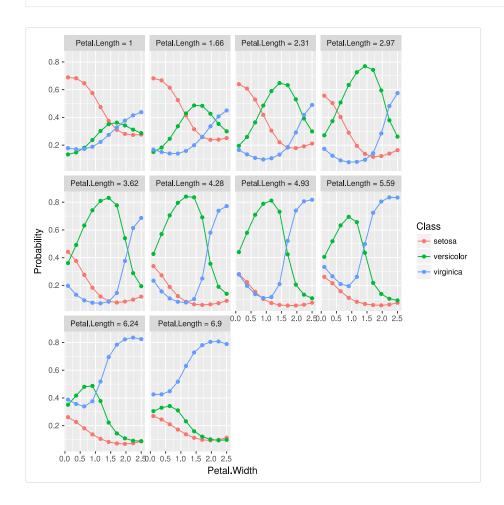
When multiple features are passed to generatePartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html) but interaction = FALSE, facetting is used to display each estimated bivariate relationship.

plotPartialDependence(pd.1st)



When interaction = TRUE in the call to generatePartialDependenceData (http://www.rdocumentation.org/packages/mlr/functions/generatePartialDependenceData.html), one variable must be chosen to be used for facetting, and a subplot for each value in the chosen feature's grid is created, wherein the other feature's partial dependences within the facetting feature's value are shown. Note that this type of plot is limited to two features.

plotPartialDependence(pd.int, facet = "Petal.Length")

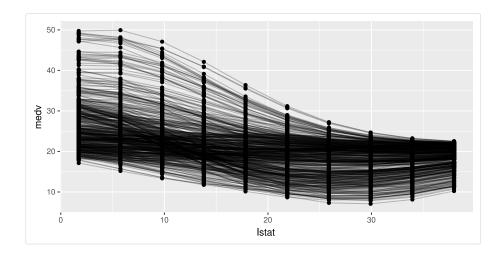


plotPartialDependenceGGVIS (http://www.rdocumentation.org/packages/mlr/functions/plotPartialDependenceGGVIS.html) can be used similarly, however, since ggvis (http://www.rdocumentation.org/packages/ggvis/) currently lacks subplotting/facetting capabilities, the argument interact maps one feature to an interactive sidebar where the user can select a value of one feature.

```
plotPartialDependenceGGVIS(pd.int, interact = "Petal.Length")
```

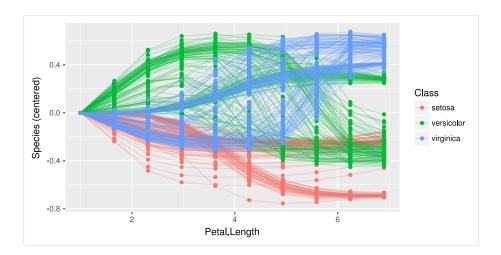
When individual = TRUE each individual conditional expectation curve is plotted.

plotPartialDependence(pd.ind.regr)



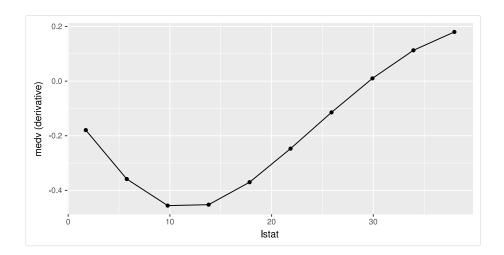
When the individual curves are centered by subtracting the individual conditional expectations estimated at a particular value of  $X_s$  this results in a fixed intercept which aids in visualizing variation in predictions made by  $\hat{f}_{X_s}^{(i)}$ .

plotPartialDependence(pd.ind.classif)



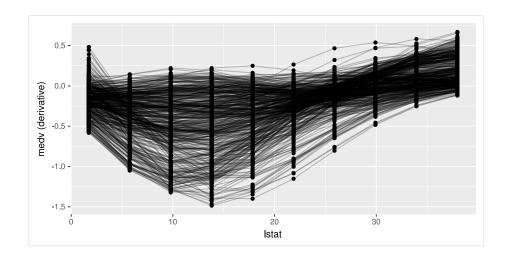
Plotting partial derivative functions works the same as partial dependence. Below are estimates of the derivative of the mean aggregated partial dependence function, and the individual partial dependence functions for a regression and a classification task respectively.

plotPartialDependence(pd.regr.der)



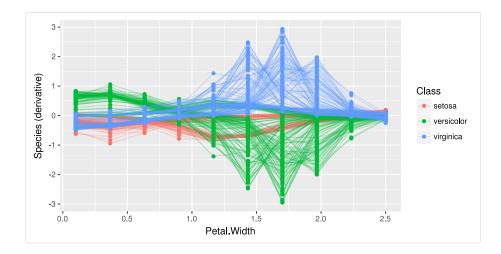
This suggests that  $\hat{f}$  is not additive in  $\boxed{\mathtt{1stat}}$  except in the neighborhood of 25.

plotPartialDependence(pd.regr.der.ind)



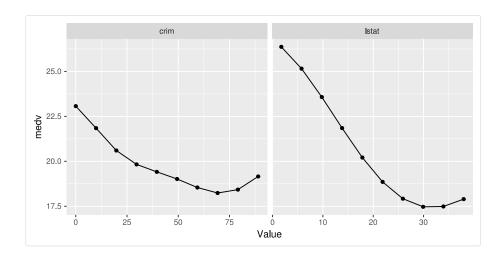
This suggests that [Petal.Width] interacts with some other feature in the neighborhood of (1.5,2) for classes "virginica" and "versicolor".

plotPartialDependence(pd.classif.der.ind)



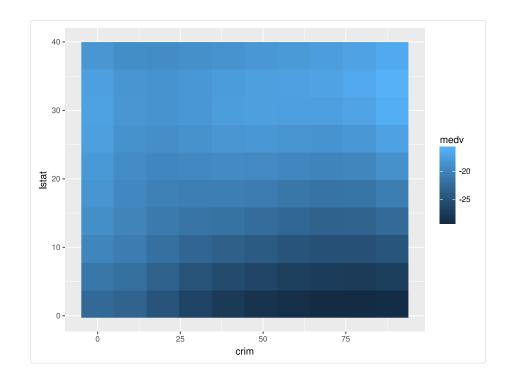
Output from generateFunctionalANOVAData (http://www.rdocumentation.org/packages/mlr/functions/generateFunctionalANOVAData.html) can also be plotted using plotPartialDependence (http://www.rdocumentation.org/packages/mlr/functions/plotPartialDependence.html).

```
fa = generateFunctionalANOVAData(fit.regr, bh.task, c("crim", "lstat"), depth = 1)
plotPartialDependence(fa)
```



Interactions can often be more easily visualized by using functional ANOVA.

```
fa.bv = generateFunctionalANOVAData(fit.regr, bh.task, c("crim", "lstat"), depth = 2)
plotPartialDependence(fa.bv, "tile")
```



Documentation built with MkDocs (http://www.mkdocs.org/).