**MLInterfaces**: towards uniform behavior of machine learning tools in R

VJ Carey, J Mar, R Gentleman

November 23, 2006

1 Introduction

We define machine learning methods as data based algorithms for prediction. Given data D, a generic machine learning procedure MLP produces a function ML = MLP(D). For data D’ with structure comparable to D, ML(D’) is a set of predictions about elements of D’.

To be slightly more precise, a dataset D is a set of records. Each record has the same structure, consisting of a set of features (predictors) and one or more predictands (classes or responses of interest, to be predicted). MLP uses features, predictands, and tuning parameter settings to construct the function ML. ML is to be a function from features only to predictands.

There are many packages and functions in R that provide machine learning procedures. They conform to the abstract setup described above, but with great diversity in the details of implementation and use. The input requirements and the output objects differ from procedure to procedure.

Our objective in **MLInterfaces** is to simplify the use and evaluation of machine learning methods by providing specifications and implementations for a uniform interface. (The `tune` procedures in e1071 also pursue more uniform interface to machine learning procedures.) At present, we want to simplify use of machine learning with microarray data, assumed to take the form of `exprSets`. The present implementation addresses the following concerns:

- simplify the selection of the predictand from `exprSet` structure;
- simplify (in fact, require) decomposition of input data into training and test set, with output emphasizing test set results;
- provide a uniform output structure.

The output structures currently supported are subclasses of a general class `MLOutput`, described in Section 3.1 below.

Several other concerns will be addressed as the project matures. Among these are:
• generic interfaces for cross-validation (exploiting native resources when available)
  
• simplified specification of criteria for outlier and doubt predictions
  
• appropriate visualizations.
  
To give a flavor of the current implementation, we perform a few runs with different machine learning tools. We will use 60 genes drawn arbitrarily from Golub’s data.

```r
> library(MLInterfaces)
> library(golubEsets)

> data(Golub_Merge)
> smallG <- Golub_Merge[200:259, ]
> smallG

ExpressionSet (storageMode: lockedEnvironment)
  assayData: 60 features, 72 samples
    element names: exprs
  phenoData
    sampleNames: 39, 40, ..., 33 (72 total)
    varLabels and varMetadata:
      Samples: Sample index
      ALL.AML: Factor, indicating ALL or AML
      ...: ...
      Source: Source of sample
        (11 total)
  featureData
    rowNames: D13627_at, D13628_at, ..., D16469_at (60 total)
    varLabels and varMetadata: none
  experimentData: use 'experimentData(object)'
    pubMedIds: 10521349
Annotation [1] "hu6800"
```

Here is how \(k\)-nearest neighbors is used to get predictions of ALL status, using the first 40 records as the training set:

```r
> krun <- knnB(smallG, "ALL.AML", trainInd = 1:40)
> krun

MLOutput instance, method= knn
Call:
  knnB(exprObj = smallG, classifLab = "ALL.AML", trainInd = 1:40)
predicted class distribution:
ALL  AML
```
summary of class assignment quality scores:

<table>
<thead>
<tr>
<th></th>
<th>Min.</th>
<th>1st Qu.</th>
<th>Median</th>
<th>Mean</th>
<th>3rd Qu.</th>
<th>Max.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

The `confuMat` method computes the confusion matrix resulting from applying the trained model to the reserved test data:

```r
> confuMat(krun)
```

<table>
<thead>
<tr>
<th>predicted</th>
<th>given ALL AML</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALL</td>
<td>18 3</td>
</tr>
<tr>
<td>AML</td>
<td>4 7</td>
</tr>
</tbody>
</table>
```

Additional parameters can be supplied as accepted by the target procedure in package `class`. To use a neural net in the same context (with fewer genes to simplify the summary below)

```r
> set.seed(1234)
> nns <- nnetB(smallG[1:10, ], "ALL.AML", trainInd = 1:40, size = 2, +    decay = 0.01, maxit = 250)
```

# weights: 25
initial value 27.327352
iter 10 value 25.018790
iter 20 value 21.799662
iter 30 value 19.267699
iter 40 value 14.859899
iter 50 value 10.836288
iter 60 value 8.196922
iter 70 value 8.182311
iter 80 value 7.381528
iter 90 value 7.291806
iter 100 value 7.204848
iter 110 value 7.185043
iter 120 value 7.159077
iter 130 value 6.803327
iter 140 value 6.779275
iter 150 value 6.778553
iter 160 value 6.778405
iter 170 value 6.778377
iter 180 value 6.778356
iter 190 value 6.778342
iter 190 value 6.778342
iter 190 value 6.778342
final value 6.778342
converged

> nns

MLOutput instance, method= nnet
a 10-2-1 network with 25 weights
inputs: D13627_at D13628_at D13630_at D13633_at D13634_at D13635_at D13636_at D13637_at D13639_at D13640_at
output(s): sampLab
options were - entropy fitting decay=0.01
Call:
  nnetB(exprObj = smallG[1:10, ], classifLab = "ALL.AML", trainInd = 1:40,
         size = 2, decay = 0.01, maxit = 250)
predicted class distribution:
ALL  AML
24   8
summary of class membership probabilities:
  [,1]
Min. 0.04531
1st Qu. 0.04531
Median 0.04531
Mean 0.26910
3rd Qu. 0.19470
Max. 0.99850

> confuMat(nns)

  predicted
given ALL AML
ALL 18 3
AML  6 5

2 Usage

The basic call sequence for supervised learning for exprSets is

methB(eset, tag, trainInd, ...)

The parameter tag is the name of the phenoData element to be used as predictand. Parameter trainInd is an integer sequence isolating the samples to be used for training. For unsupervised learning,
methB(ezet, k, height, ...)

The idea here is that one may specify a number k of clusters, or a height of a clustering tree that will be cut to form clusters from the eset samples. Note that there is no training/test dichotomy for clustering at this stage.

The RObject method will access the fit object from the basic procedure. Thus, returning to the nnetB invocation above, we have

```r
> summary(RObject(nns))
```

a 10-2-1 network with 25 weights

options were - entropy fitting decay=0.01

b->h1  i1->h1  i2->h1  i3->h1  i4->h1  i5->h1  i6->h1  i7->h1  i8->h1  i9->h1
 0.00  0.02 -0.17  0.07  0.03 -0.02 -0.05 -0.06 -0.07  0.01
i10->h1
  0.00

b->h2  i1->h2  i2->h2  i3->h2  i4->h2  i5->h2  i6->h2  i7->h2  i8->h2  i9->h2
 0.00 -0.10  0.12 -0.10  0.16  0.08  0.21  0.00 -0.10  0.00
i10->h2
  0.03

b->o  h1->o  h2->o
 0.59 -3.64  5.94

which is the customary nnet summary. This also gives access to visualization.

```r
> ags <- agnesB(smallG, k = 4, height = 0, stand = FALSE)
```

```r
> plot(RObject(ags), which.plot = 2)
```
3 Classes

The S4 class structure is based on a few observations. First, there are two basic types of task covered in machine learning, ‘supervised’ (MLP uses known classes and ML returns predictand instances) and ‘unsupervised’ (MLP groups data based on features, no predictand data assumed; ML can tell which group D’ is closest to). Second, there is an important concept of ‘quality’ of prediction or clustering events, and it will be important to allow flexible representation of different approaches to quality measurement by machine learning procedures. Third, there are various things that one always wants access to, regardless of the underlying MLP (call information, R object constituting the ‘fit’ to the training data). This leads to general classes MLOutput, which collects the most general information of interest, MLLabel, which represents predictand or clustergroup information, and MLScore, which represents quality information. Classes classifOutput and clustOutput manage the results of supervised and unsupervised learning respectively.


3.1 MLOutput

Extended by all machine learning output containers.

> getClass("MLOutput")

Slots:

Name: method RObject call distMat
Class: character ANY call dist

Known Subclasses: "classifOutput", "clustOutput"

3.1.1 MLLabel

Identifies the results of machine learning labeling events, either in the form of class labels or integer cluster indices.

> getClass("MLLabel")

Virtual Class

No Slots, prototype of class "S4"

Known Subclasses: "predClass", "groupIndex"

3.1.2 MLScore

Identifies quality information about classification or clustering events. This can range from a scalar (agglomeration coefficient, not yet used) to a vector (vote proportions in knn) to a matrix (posterior probabilities of class assignments) to an array (pamr thresholded posteriors).

> getClass("MLScore")

Virtual Class

No Slots, prototype of class "S4"

Known Subclasses: "probMat", "probArray", "membMat", "qualScore", "silhouetteVec"
3.2 classifOutput

Container for classification results.

> getClass("classifOutput")

Slots:

Name: predLabels predScores trainInds allClass method RObject
Class: MLLabel MLScore integer character character ANY

Name: call distMat
Class: call dist

Extends: "MLOutput"

3.3 clustOutput

Container for clustering results.

> getClass("clustOutput")

Slots:

Name: clustIndices clustScores method RObject call
Class: MLLabel MLScore character ANY call

Name: distMat
Class: dist

Extends: "MLOutput"

4 A sketch of a ‘doubt’ computation

The nnet function returns a structure encoding predicted probabilities of class occupancy. We will use this to enrich the nnetB output to include a “doubt” outcome. As written this code will handle a two-class outcome; additional structure emerges with more than two classes and some changes will be needed for such cases.

First we obtain the predicted probabilities (for the test set) and round these for display purposes.

> predProb <- round(nns@predScores, 3)

We save the true labels and the predicted labels.
> truth <- as.character(smallG$ALL.AML[-c(1:40)])
> simpPred <- predict(RObject(nns), newdata = data.frame(t(exprs(smallG)[1:10, +  -c(1:40)])), type = "class")

We create a closure that allows boundaries of class probabilities to be specified for assertion of “doubt”:

> douClo <- function(pprob) function(lo, hi) pprob > lo & pprob < + hi

Evaluate the closure on the predicted probabilities, yielding a function of two arguments (lo, hi).

> smallDou <- douClo(predProb)

Now replace the labels for those predictions that are very close to .5.

> douPred <- simpPred
> douPred[smallDou(0.48, 0.52)] <- "doubt"

The resulting modified predictions are in the fourth column:

> mm <- cbind(predProb, truth, simpPred, douPred)
> mm

<table>
<thead>
<tr>
<th></th>
<th>truth</th>
<th>simpPred</th>
<th>douPred</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>&quot;0.643&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;AML&quot;</td>
</tr>
<tr>
<td>8</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>9</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>10</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>11</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>12</td>
<td>&quot;0.94&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;AML&quot;</td>
</tr>
<tr>
<td>13</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>14</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>15</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>16</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>17</td>
<td>&quot;0.999&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;AML&quot;</td>
</tr>
<tr>
<td>18</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>19</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>20</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>21</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>22</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>23</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>24</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
<tr>
<td>25</td>
<td>&quot;0.045&quot;</td>
<td>&quot;ALL&quot;</td>
<td>&quot;ALL&quot;</td>
</tr>
</tbody>
</table>
> table(mm[, "truth"], mm[, "simpPred"])

    AML
   ALL 18  3
   AML  6  5

> table(mm[, "truth"], mm[, "douPred"])

    AML
   ALL 18  3
   AML  6  5