PivotalR: A Package for Machine Learning on Big Data

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Abstract PivotalR is an R package that provides a front-end to PostgreSQL and all PostgreSQL-like databases like Pivotal Inc.'s Greenplum Database (GPDB), HAWQ Pivotal Inc. (2013a). When running on the products of Pivotal Inc., **PivotalR** utilizes the full power of parallel computation and distributive storage embedded in Greenplum Database or HAWQ, and thus gives the normal R user access to big data. **PivotalR** also provides the R wrapper for MADlib. MADlib is an open-source library for scalable in-database analytics. It provides data-parallel implementations of mathematical, statistical and machine-learning algorithms for structured and unstructured data. Thus **PivotalR** also enables the user to apply machine learning algorithms onto big data.

Introduction

In recent years, Big Data has become an important research topic and a very realistic problem in industry. The amount of data that we need to process is exploding, and the ability of analyzing big data has become the key factor in competition.

The package Pivotal R Pivotal Inc. (2013c) provides an R front-end for R users to access big data stored in distributive databases or Hadoop distributive file system (HDFS) The Apache Software Foundation (2013).

PivotalR also provides a wrapper for MADlib Pivotal Inc. (2013b), which is an open-source library of scalable in-database machine learning algorithms. Actually **PivotalR** offers more than what MADlib has. It adds functionalities that do not exist in MADlib, for example, the support for categorical variables.

PivotalR is especially useful for users who are not familiar with SQL language, because the functions and syntax that it defines for the manipulation of tables stored in the distributive database are very similar to those for data.frame manipulation defined natively in R. Thus the learning curve for the package is very smooth.

PivotalR is also very useful for users who are familiar with SQL language, because it brings the graphical and analytical powers of R to the processing of big data stored in databases.

PivotalR is contributed to the open-source community by the Predictive Analytics Team at Pivotal Inc. Although the users need to have a distributive database system installed, for example the Greenplum Database or HAWQ, in order to gain the power of distributive storage and parallel computation, **PivotalR** also supports the open-source database system PostgreSQL. Therefore **PivotalR** benefits normal R users by providing an easy-to-access interface for manipulating data tables stored in PostgresISQL database system and a combination of the powers of R and MADlib, which lets the user directly apply machine learning algorithms onto data stored in databases.

It is worth mentioning that **PivotalR** provides the access to data stored on HDFS by supporting HAWQ, which is the SQL query engine on HDFS created by Pivotal Inc.

PivotalR minimizes the amount of data transferred between the database and R. The user manipulates the data from R but the data itself stays in the database. Thus the user does not need to worry about the restriction of memory size even if the data size is very big.

At the time of writing, the version of PivotalR on CRAN is 0.1.4.

In this paper, we briefly introduce the usage of **PivotalR**. First in the next section we explain the architecture of **PivotalR**. Then we use various examples to illustrate the usage and work flow of **PivotalR**.

Architecture of PivotalR

As is shown in Fig. (1), **PivotalR** connects to the database through the **RPostgreSQL** Conway et al. (2013) package. However, **PivotalR** does not directly call the functions in RPostgreSQL. Instead we create an abstraction layer to wrap the functions of RPostgreSQL, and the access to the database is by calling the functions in the abstraction layer, which then call the functions in RPostgreSQL. This design makes it easier to add supports for other data storage platforms in the future. Right now, **PivotalR**

only supports the connection to PostgreSQL, GPDB (Greenplum Database) and HAWQ. Through HAWQ, **PivotalR** can access the big data stored on HDFS.

In the future, **PivotalR** will add supports to other DBMS, Pivotal HD (Hadoop created by Pivotal Inc.) and Hadoop (MapReduce), but we have not decided about how to do that. This is why there are question markers in Fig. (1).

Built upon the table operations are the MADlib function wrappers and other functions, which will be covered in the subsequent sections.

A graphical user interface using the **shiny** RStudio Inc. (2013) package is also implemented. Right now it only provides the graphical interface to the MADlib wrapper functions, but will provide the graphical access to all functionalities of **PivotalR** in the future.

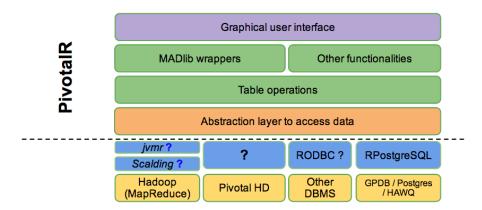


Figure 1: The structure of **PivotalR**. **PivotalR** accesses the data storage through an abstraction layer which wraps the functions that can directly access the database. Other types of data storages will be supported in the future. Right now it only supports connections to PostgreSQL, GPDB and HAWQ. Table operations functions are built upon the data accessing layer. They have the exact same interface as R's "data.frame" operation functions. MADlib function wrappers and other functions are built upon the table operations. The graphical user interface makes the package easier to use.

It is worth explaining more about how **PivotalR** operates on the tables. Before everything, the user needs to create a "db.data.frame" object, which is just a wrapper of the table. Any operation on this object is translated into an SQL query string. However, the SQL query is not executed at this point, and is instead stored in an object of class "db.Rquery" in R. When the user wants to execute the operation, he can call the function preview or lookat to execute the operation and load part or all of the results into memory to view. The user can also choose to use as.db.data.frame to execute the SQL query and save the result into a new table. This design gives the user the freedom to choose when to load data into memory or create tables to store intermediate data in the process of a calculation. It also avoids the risk of accidentally loading big data into memory.

In order to realize the above design, we use a class hierarchy shown in Fig. (2). **PivotalR** uses S4 object-oriented programming extensively. All objects that are related to the data in the database belong to subclasses of an abstract class named "db.object".

As has been mentioned, the class "db.data.frame" is a wrapper of data objects stored in the connected database. When it is created by the command "db.data.frame", no actual data stored in the data table in the database is transferred from the database to R. This object just contains some basic information about the data object in the database, such as dimensions and column names. "db.data.frame" has two sub-classes, "db.table" and "db.view", which are wrappers for tables and views respectively.

Here, the command db.connect in the abstraction layer is used to connect to one or multiple

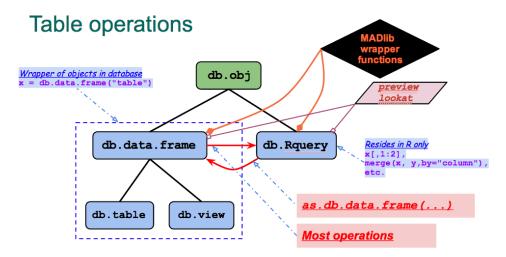


Figure 2: The class hierarchy of PivotalR.

databases. It has an optional parameter that let the user select which package he wants to use to connect to the databases, although only **RPostgreSQL** is allowed right now. The returned value of db.connect is an integer which represents the database connection. **PivotalR** can connect to multiple databases at the same time. Thus it is possible to train a machine learning model using the data from database 1 and make predictions using the data from database 2. One can use db.disconnect to disconnect a connection and db.list to list all active connections.

Any operation on an object of the class "db.data.frame" produces an object of the class "db.Rquery". An object of the class "db.Rquery" resides entirely on the R side, and is a wrapper of operations on a "db.data.frame" object. Most operations on a "db.Rquery" object produces another "db.Rquery" object. Essentially, a "db.Rquery" object is just a string of SQL query, which can be viewed using the command content. The command as.db.data.frame creates a table in the database using the results of the SQL query contained in a "db.Rquery" object and then creates a "db.data.frame" wrapper that points to this table.

preview (or its alias lookat) transfers the data from the database into R's memory. By default it fetches 100 rows of data from the table in the database and convert the data into "data.frame" in R.

```
> lookat (x, 10)
  id sex length diameter height whole shucked viscera shell rings
       M 0.440
                  0.365 0.125 0.5160 0.2155 0.1140 0.155
          0.545
                   0.425 0.125 0.7680 0.2940 0.1495 0.260
3
  12
       М
          0.430
                   0.350 0.110 0.4060
                                      0.1675 0.0810 0.135
4
  16
       Μ
          0.500
                  0.400 0.130 0.6645
                                      0.2580 0.1330 0.240
                                                              12
5
  20
       Μ
          0.450
                   0.320 0.100 0.3810
                                      0.1705 0.0750 0.115
                                                               9
6
  24
       F
          0.550
                   0.415 0.135 0.7635 0.3180 0.2100 0.200
                                                               9
  28
       M 0.590
                   0.445 0.140 0.9310 0.3560 0.2340 0.280
                                                              12
       F
                   0.560 0.165 1.6390 0.6055 0.2805 0.460
8
  32
          0.680
                                                              15
       M 0.465
                   0.355 0.105 0.4795 0.2270 0.1240 0.125
  36
                                                               8
10 40
                   0.290 0.090 0.3275 0.1340 0.0860 0.090
       M 0.355
```

The MADlib wrappers can be applied onto both "db.data.frame" and "db.Rquery" objects. When a MADlib wrapper function is applied onto a "db.Rquery" object, a temporary table is created using as.db.data.frame since MADlib itself is an in-database library and we have to convert "db.Rquery" into an object inside the database so that we could apply MADlib functions onto it. This temporary table is dropped after the computation is done.

The design of **PivotalR** minimizes the amount of data that needs to be transferred between the database and R. The only function that transfers data from the database is "preview (or its alias lookat).

Manipulation of Data Tables in Database

As has been mentioned, **PivotalR** overloads many methods that operate on "data.frame", and thus let the operations on the "db.obj" objects mimic those on "data.frame" as much as possible.

```
> x <- db.data.frame ("abalone")</pre>
> dim(x)
[1] 4177
> names (x)
 [1] "id"
                "sex"
                           "length"
                                      "diameter" "height"
                                                            "whole"
[7] "shucked" "viscera" "shell"
                                      "rings"
> x$rings <- x$rings + 2 / 3
> x \cdot - (x \cdot + x[['length']]) < 10
> content(x)
[1] "select id" as id", sex" as sex", length" as length",
diameter as diameter, height as height, whole as whole,
shucked as shucked, viscera as viscera, shell as shell,
(rings)::double precision + 0.666666666666666667 as rings,
(((rings)::double precision + 0.6666666666667)::double precision
+ (length)::double precision < 10 as newCol from abalone
```

Here content displays the SQL query stored in the "db.Rquery". The quotes inside the SQL query is used to deal with column or table names with special characters. x was originally a "db.data.frame" object, but became a "db.Rquery" object by the operation xrings < -xrings + 2 / 3.

The operations on "db.obj" objects mimic those on "data.frame". However, there is important difference between "db.obj" and "data.frame".

The rows of a "data.frame" object have an intrinsic order, which makes the operations that involve two "data.frame" objects easier to define. For example, it is straightforward to define the subtraction of two columns of two different "data.frame" objects by matching the order of the rows as long as they have the same number of rows.

On the other hand, the tables in the database do not have intrinsic order for the rows. Thus, most operations like subtraction, addition etc. can only be defined for columns belonging to the same table. However, this is usually not a problem. Whenever the user wants to do some operation that involves two tables, he/she should first call the function merge to create a new table from the two tables and at the same time explicitly specify how to match the rows of the two different tables. Then, the user can easily do operations on the new table. While R's "data.frame" implicitly uses the intrinsic order of the rows to match the rows from two different tables, this needs to be explicitly done for "db.data.frame" objects. For example,

```
> x <- db.data.frame("abalone")</pre>
> y <- db.data.frame("abalone")</pre>
> z <- merge(x, y, by = NULL) # cross join two tables
> names(z)
 [1] "id_x"
                   "sex_x"
                                "length_x"
                                              "diameter_x" "height_x"
 [6] "whole_x"
                               "viscera_x"
                                              "shell_x"
                                                           "rings_x"
                   "shucked_x"
                                "length_y"
                                              "diameter_y" "height_y"
[11] "id_y"
                   "sex_y"
                   "shucked_y" "viscera_y"
[16] "whole_y"
                                              "shell_y"
                                                           "rings_y"
> z$sex_x == z$sex_y # This is a db.Rquery object
```

The data frame 'abalone' is lazy-loaded in **PivotalR**. It is used as an example data here. One can use as . db . data . frame to transfer this data set into a table in the database and at the same time create a wrapper for the table

```
> x <- as.db.data.frame(abalone, conn.id=1) The data in the data.frame abalone is stored into the table in database madlib on localhost !
```

All the subsequent operations will be applied onto the table wrapper x. A sample of the data is shown in the following, where sort is used to create a sorting operation on the original table.

```
> lookat(sort(x, FALSE, x$id), 10) # load 10 rows of the sorted data
   id sex length diameter height whole shucked viscera shell rings
        M 0.455
                    0.365 0.095 0.5140 0.2245 0.1010 0.150
                                                                   15
                    0.265 0.090 0.2255 0.0995 0.0485 0.070
2
    2
        M 0.350
                                                                    7
                    0.420 0.135 0.6770 0.2565 0.1415 0.210
        F 0.530
    3
       M 0.440
                    0.365 \quad 0.125 \ 0.5160 \quad 0.2155 \quad 0.1140 \ 0.155
                                                                   10
                     0.255 \quad 0.080 \ 0.2050 \quad 0.0895 \quad 0.0395 \ 0.055 
       I 0.330
                                                                    7
       I 0.425
                    0.300 0.095 0.3515 0.1410 0.0775 0.120
       F 0.530
                    0.415 0.150 0.7775 0.2370 0.1415 0.330
                                                                   20
```

```
8 8 F 0.545 0.425 0.125 0.7680 0.2940 0.1495 0.260 16
9 9 M 0.475 0.370 0.125 0.5095 0.2165 0.1125 0.165 9
10 10 F 0.550 0.440 0.150 0.8945 0.3145 0.1510 0.320 19
```

At last, I want to reiterate that all these operations done on "db.data.frame" are not executed immediately. Instead a "db.Rquery" object is produced, which the user can choose to convert into a real table using as.db.data.frame.

MADlib Wrapper Functions

In the next, we show some examples of MADlib wrapper functions. As is shown in Fig. (2), all MADlib wrapper functions can be applied onto "db.obj" objects. Because the connection information is already contained in "db.obj" objects, we do not need to specify conn.id in the MADlib wrapper functions.

First, we show several examples of linear regression. Basically, PivotalR's madlib.lm uses the same formula syntax as lm. Because MADlib's linear regression supports fitting separate linear regression models on sub-groups of the data, which are grouped by one or multiple columns, madlib.lm allows | in the formula, which means that the model is fit on a subset of the data conditioned on the value of the variables after |.

```
> ## fit one different model to each group of data with the same sex > fit <- madlib.lm(rings \sim . - id | sex, data = x)
```

sex has 3 distinct values, and thus fit is a list of 3 elements. Each element is the linear regression model for a subset of the data. The mean square error can be easily computed

We can plot a random sample of the fitting values together with the real values, as is shown in Fig. (3). We can also select one model from the fitting result to plot, as is shown in the comments of the following snippets.

```
> ## plot the result
> ap <- cbind(x$rings, predict(fit, x)) # combine two columns
> plot(lookat(sort(ap, FALSE, NULL), 100)) # plot a random sample
> ## ap <- cbind(x$rings[x$sex == "I"], predict(fit[[1]], x[x$sex == "I",]))
> ## plot(lookat(sort(ap, FALSE, NULL), 100)) # plot a random sample
```

The support to categorical variables is done through "as.factor", as is shown in the next example.

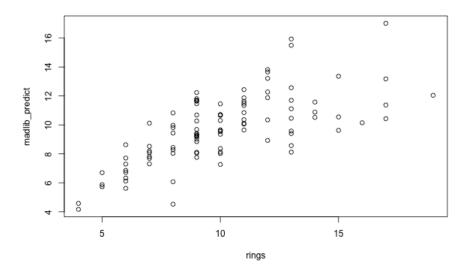


Figure 3: The sample plot

```
height
            10.76154
                        1.53620
                                 7.0053 2.861e-12 ***
whole
             8.97544
                        0.72540 12.3730 1.469e-34 ***
shucked
            -19.78687
                        0.81735 -24.2086 2.988e-121 ***
viscera
           -10.58183
                        1.29375 -8.1792 3.757e-16 ***
shell
             8.74181
                        1.12473
                                 7.7723 9.639e-15 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
R-squared: 0.5378844
Condition Number: 137.2694
```

In the next example, we use the bootstrap aggregate method to fit a linear model to the data.

Just like glm in stats R Core Team (2013) package, PivotalR provides madlib.glm, which can do both linear and logistic regressions. The usage is similar to glm. Please refer to PivotalR manual Pivotal Inc. (2013c) for details.

Support for Array Columns

Besides the lacking of order, there is one more difference between "data.frame" and tables in a database. The value of a column of a table can be an array. **PivotalR** has the full support for such array columns, as is shown in the next example.

```
8 400 150 3761 9.5
                             70
                                   1 15
        121
             113 2234 12.5
                             70
                                   2 26
            215 4615 14.0
                                   1 10
     8
        360
                             70
        304 193 4732 18.5
                             70
                                   1 9
             95 2228 14.0
                                   3 25
     4 113
                             71
     6 250
             88 3302 15.5
                             71
                                  1 19
     8 351 153 4154 13.5
                             71
                                  1 14
     8 318 150 4096 13.0
                                   1 14
> madlib.lm(y \sim x, data = z)
MADlib Linear Regression Result
Call:
madlib.lm(formula = y \sim x, data = z)
Coefficients:
             Estimate Std. Error t value
                                             Pr(>|t|)
(Intercept) -17.218435
                       4.644294 -3.7074 2.402e-04 ***
x[1]
            -0.493376
                        0.323282 -1.5261 1.278e-01
                        0.007515 2.6474 8.445e-03 **
x[2]
             0.019896
x[3]
            -0.016951
                        0.013787 -1.2295 2.196e-01
                        0.000652 -9.9288 7.883e-21 ***
x[4]
            -0.006474
                        0.080576
x[5]
             0.750773
                        0.050973 14.7288 3.069e-39 ***
x[6]
                        0.278136 5.1275 4.666e-07 ***
x[7]
             1.426140
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R-squared: 0.8214781
```

Handling of NULL Values

Condition Number: 85850.33

PivotalR makes it very easy to filter NULL values from a table. Here we show an example using the data "null.data" comes with **PivotalR**. 'null.data' has lots of NULL values, and a direct linear regression on the data will fail because MADlib does not handle NULL values right now. However, we can easily filter out all the NULL values.

```
> delete("null_data", conn.id = 2)
[1] TRUE
> w <- as.db.data.frame(null.data, "null_data", conn.id = 2)</pre>
The data in the data.frame null.data is stored into the table null_data in database madlib on localhost!
> dim(w)
[1] 67126
              10
> lookat(w, 10)
   sf_mrtg_pct_assets ris_asset lncrcd lnauto lnconoth lnconrp intmsrfv
                 31.62
                           208596
                                       0
                                              NA
                                                    18260
                                                                44
2
                 20.66
                           34647
                                       0
                                              NA
                                                     2997
                                                                 0
                 14.95
                           160175
                                                    15164
3
                                              NA
                 17.49
                          117398
                                              NA
                                                    12365
                                                                 0
5
                 35.59
                           233592
                                       0
                                              NA
                                                     6261
                                                               151
                 11.57
                           166387
                                       0
                                             NA
                                                    36356
                                                                 0
7
                 10.56
                           102891
                                       0
                                             NA
                                                     6311
                                                                 0
                                                                          0
8
                  6.05
                           30138
                                       0
                                             NA
                                                     2664
                                                                 0
                                                                           0
9
                 14.53
                         1615727
                                       0
                                             NA
                                                    80829
                                                              1106
                                                                         105
10
                 12.88
                            83090
                                             NA
                                                    11815
                                                                 0
   lnrenr1a lnrenr2a lnrenr3a
1
         NA
                   NA
                            NA
2
         NA
                   NA
                             NA
3
         NA
                   NA
                             NA
4
         NA
                   NA
                             NA
```

NA

NA

NA

5

```
6
        NA
                 NA
                          NA
7
        NA
                 NA
                         NA
8
        NA
                 NA
                         NA
        NA
                 NA
                         NA
10
        NA
                         NA
> db.objects("null", conn.id = 2)
[1] "madlibtestdata.credit_nulls"
                                        "madlibtestdata.rf_golf_nullclass"
[3] "madlibtestdata.rf_nursery_nullclass" "madlibtestdata.table_has_null"
[5] "public.null_data"
> ## madlib.lm(sf_mrtg_pct_assets ~ ., data = w) # will fail
> for (i in 1:10) w <- w[!is.na(w[i]),] # filter NULL values
[1] 6789
> madlib.lm(sf_mrtg_pct_assets ~ ., data = w)
MADlib Linear Regression Result
madlib.lm(formula = sf_mrtg_pct_assets ~ ., data = w)
Coefficients:
             Estimate Std. Error t value
                                               Pr(>|t|)
(Intercept) 1.528e+01 1.471e-01 103.90694 0.000e+00 ***
            1.602e-08 1.141e-08 1.40440 1.602e-01
ris asset
          -1.608e-07 7.725e-08 -2.08170 3.741e-02 *
lncrcd
          -3.871e-07 3.447e-07 -1.12301 2.615e-01
lnauto
lnconoth -7.498e-07 4.370e-07 -1.71559 8.628e-02
          7.575e-08 1.229e-06 0.06165 9.508e-01
lnconrp
intmsrfv 8.609e-06 1.790e-06 4.81005 1.542e-06 ***
lnrenr1a -4.827e-06 3.837e-05 -0.12580 8.999e-01
           1.358e-04 2.359e-05 5.75605 8.986e-09 ***
lnrenr2a
lnrenr3a -3.133e-05 4.273e-06 -7.33355 2.502e-13 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R-squared: 0.01083685
```

Quickly Creating Prototypes of Machine Learning Algorithms

One of the goals of **PivotalR** is to help data scientists quickly create prototypes for parallel machine learning algorithms that can run in distributive database. Although **PivotalR** is still at its early stage, we already invest some effort into this. The idea is to implement some basic operations that forms the build blocks for most machine learning algorithms.

For example, we implemented the function crossprod, which computes the operation X^TY . X and Y are wrappers created by "db.data.frame" for tables that represent matrices. X has M rows (observations) and N columns (features). The assumption here is that M can be very large but the number of features N is small. Thus results of X^TX and X^TY are both small and can be loaded into memory for further calculations. The big data computation only involves the computations of X^TX and X^TY in the database.

```
## linear regression
linregr <- function (x, y)

a <- crossprod (x)
b <- crossprod (x, y)
solve (lookat (a)) %*% lookat(b)

linregr (db.array(1, x[,-c (1,2,10)]), x[["rings"]])</pre>
```

Another example is the implementation of PCA for a matrix Z. Again we assume that the number

Condition Number: 37854014



Figure 4: Display the summary of a table in the graphical interface.

of columns n is not large and the product Z^TZ is small enough to be loaded into memory. **PivotalR** implements scale, which is used together with crossprod in this example.

```
## PCA
## compute all eigenvectors in parallel
## can be used for tables with features < 1000
pca <- function (x, center = TRUE, scale = FALSE)</pre>
  y <- scale(x, center = center, scale = scale) # centering and scaling
 z \leftarrow as.db.data.frame(y, verbose = FALSE) # create an intermediate table to save computation
  m <- lookat(crossprod(z)) # one scan of the table to compute Z^T \star Z
  d <- delete(z) # delete the intermediate table</pre>
  res <- eigen(m) # only this computation is in R
  n \leftarrow attr(y, "row.number") # save the computation to count rows
  ## return the result
  list(val = sqrt(res$values/(n-1)), # eigenvalues
  vec = res$vectors, # columns of this matrix are eigenvectors
  center = attr(y, "scaled:center"),
  scale = attr(y, "scaled:scale"))
dat <- db.data.frame("madlibtestdata.pca_mat_600_100", conn.id = 2)</pre>
q <- pca(dat[,-1])</pre>
```

GUI of PivotalR

As a front-end to both the database and MADlib, **PivotalR** also provides a graphical user interface (GUI) to let users that are not familiar with data science have an easy access to many of the functionalities. The GUI is written using the package **shiny**, which provides a very nice web application framework to create graphical user interface.

The GUI is launched by the command pivotalr after the connection to the databases have been created. Fig. 4 and Fig. 5 show the graphical user interface. Fig. 4 shows the screen shot for the summary of various properties for all columns of a table. The actual computation is done through MADlib's "summary" function, which has a wrapper function madlib.summary in PivotalR. Fig. 5 shows the computation result of linear regression. The actual computation is done through MADlib's linregr_train function, which has a wrapper function madlib.lm.

The GUI of **PivotalR** is based upon the package **shiny**, which is a web application framework. Therefore the command pivotalr launches a web application. One can run the GUI on the server and connect to it using his web browser.

The GUI of PivotalR is still at its early development stage. Many functionalities, especially the

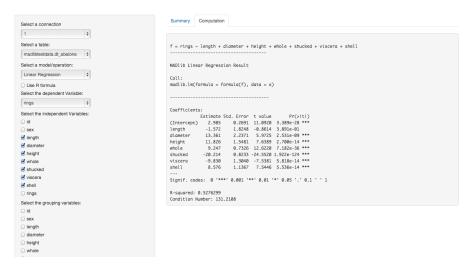


Figure 5: Display the result of linear regression in the graphical interface.

various operations on data tables, cannot be done through GUI. However, we expect to improve the GUI gradually in the future releases.

Summary

Here we introduced **PivotalR**, a package created by Pivotal Inc. This package provides an R front-end to PostgreSQL and all PostgreSQL-like databases like Pivotal Inc.'s Greenplum Database (GPDB), HAWQ. **PivotalR** allows the user to manipulate tables in database from within R. It also provides wrapper functions for MADlib, which is an in-database machine learning library. **PivotalR** implements the support for array columns and NULL handling. It also helps the user quickly create prototypes of machine learning algorithms. A graphical user interface based on shiny is also implemented. In general, **PivotalR** gives the user the access to big data stored in databases and an easy-to-use machine learning toolkit.

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