Generalized Linear Modeling with H2O's R Package

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1 Introduction

This document describes Generalized Linear Model implementation on H2O platform, list of supported features and how to use them from R.

2 What is H2O?

H2O is fast scalable open-source machine learning and deep learning for Smarter Applications. With H2O, enterprises like PayPal, Nielsen, Cisco and others can use all of their data without sampling and get accurate predictions faster. Advanced algorithms, like Deep Learning, Boosting, and Bagging Ensembles are readily available for application designers to build smarter applications through elegant APIs. Some of our earliest customers have built powerful domain-specific predictive engines for Recommendations, Customer Churn, Propensity to Buy, Dynamic Pricing and Fraud Detection for the Insurance, Healthcare, Telecommunications, AdTech, Retail and Payment Systems.

Using in-memory compression techniques, H2O can handle billions of data rows in-memory, even with a fairly small cluster. The platform includes interfaces for R, Python, Scala, Java, JSON and Coffeescript/JavaScript, along with a built-in web interface, Flow, that make it easier for non-engineers to stitch together complete analytic workflows. The platform was built alongside (and on top of) both Hadoop and Spark Clusters and is typically deployed within minutes.

H2O implements almost all common machine learning algorithms, such as generalized linear modeling (linear regression, logistic regression, etc.), Naïve Bayes, principal components analysis, time series, k-means clustering and others. H2O also implements best-in-class algorithms such as Random Forest, Gradient Boosting and Deep Learning at scale. Customers can build thousands of models and compare them to get the best prediction results.

H2O is nurturing a grassroots movement of physicists, mathematicians, computer and data scientists to herald the new wave of discovery with data science. Academic researchers and Industrial data scientists collaborate closely with our team to make this possible. Stanford university giants Stephen Boyd, Trevor Hastie, Rob Tibshirani advise the H2O team to build scalable machine learning algorithms. With 100s of meetups over the past two years, H2O has become a word-of-mouth phenomenon growing amongst the data community by a 100-fold and is now used by 12,000+ users, deployed in 2000+ corporations using R, Python, Hadoop and Spark.

Try it out

H2O offers an R package that can be installed from CRAN. H2O can be downloaded at www.h2o.ai/download.

Join the community

Connect with h2ostream@googlegroups.com and https://github.com/h2oai to learn about our meetups, training sessions, hackathons, and product updates.

Learn more about H2O

Visit www.h2o.ai.

3 What is GLM?

Generalized linear models (GLM) are the workhorse for most predictive analysis use cases. GLM can be used for both regression and classification, it scales well to large datasets, and is based on solid statistical background. It is a generalization of linear models, allowing for modeling of data with exponential distributions and for categorical data (classification). GLM models are fitted by solving the maximum likelihood optimization problem.

3.1 GLM on H2O

H2O's GLM algorithm fits the generalized linear model with elastic net penalties. The model fitting computation is distributed, extremely fast, and scales extremely well for models with a limited number (~ low thousands) of predictors with non-zero coefficients. The algorithm can compute models for a single value of a penalty argument or the full regularization path, similar to the glmnet package for R (refer to Regularization Paths for Generalized Linear Models via Coordinate Descent by Friedman et. al). H2O's GLM fits the model by solving following problem:

$$\min_{\beta} \frac{1}{N} log - likelihood(family, \beta) + \lambda(\alpha\|\beta\|_1 + \frac{1-\alpha}{2}\|\beta\|_2^2)$$

The elastic net parameter α controls the penalty distribution between L1 and L2 penalty. The range is any value between 0 and 1. When $\alpha = 0$, we have no L1 penalty and the problem becomes ridge regression. If $\alpha = 1$, there is no L2 penalty and we have lasso.

The main advantage of an L1 penalty is that with sufficiently high λ, it produces a sparse solution; the L2-only penalty does not reduce coefficients to exactly 0. The two penalties also differ in the case of correlated predictors. The L2 penalty shrinks coefficients for correlated columns towards each other, while the L1 penalty will pick one and drive the others to zero. Using the elastic net argument α, you can combine these two behaviors. It is also useful to always add a small L2 penalty to increase numerical stability.

Similarly to the methods discussed in Regularization Paths for Generalized Linear Models via Coordinate Descent by Friedman et. al, H2O can compute the full regularization path, starting from null-model (maximum penalty) going down to minimally penalized model. This search is made efficient by employing strong-rules as described in Strong Rules for Discarding Predictors in Lasso-type Problems by Bien et. al to filter out inactive coefficients (coefficients pushed to zero by penalty). Computing the full regularization path is useful in that it gives more insight about the importance of individual coefficients and quality of the model while allowing selection of the optimal amount of penalization for the given problem and data.

3.1.1 Summary of features

In summary, H2O's GLM functionalities include:

- fits generalized linear model with elastic net penalty
- supported GLM families include Gaussian, Binomial, Poisson and Gamma
- efficient handling of categorical variables
- efficient computation full regularization path
- efficient distributed n-fold cross validation
- distributed grid search over elastic-net parameter α

- upper and lower bounds for coefficients
- proximal operator interface

4 Installation

You can load the latest CRAN H2O package by running:

```
> install.packages("h2o")
```

Alternatively, you can (and should for this tutorial) download the latest H2O build by following the "Install in R" instructions in the H2O download table:

http://s3.amazonaws.com/h2o-release/h2o/master/latest.html.

Open your R Console and run the following to install the latest H2O build in R:

```
# The following two commands remove any previously installed H2O packages for R.
if ("package:h2o" %in% search()) { detach("package:h2o", unload=TRUE) }
if ("h2o" %in% rownames(installed.packages())) { remove.packages("h2o") }

# Next, we download packages that H2O depends on.
if (! ("methods" %in% rownames(installed.packages()))) { install.packages("methods") }
if (! ("statmod" %in% rownames(installed.packages()))) { install.packages("statmod") }
if (! ("stats" %in% rownames(installed.packages()))) { install.packages("stats") }
if (! ("graphics" %in% rownames(installed.packages()))) { install.packages("graphics") }
if (! ("RCurl" %in% rownames(installed.packages()))) { install.packages("RCurl") }
if (! ("rjson" %in% rownames(installed.packages()))) { install.packages("rjson") }
if (! ("tools" %in% rownames(installed.packages()))) { install.packages("tools") }
if (! ("utils" %in% rownames(installed.packages()))) { install.packages("utils") }

# Now we download, install and initialize the H2O package for R (replacing
the * with the latest version number obtained from the H2O download page)
install.packages("h2o", type="source", repos=(c("http://h2o-release.s3.amazonaws.com/h2o/master/*/R")))
library(h2o)
localH2O = h2o.init(nthreads = -1)
```

To launch on a single node, initialize H2O on all the cores of your machine with

```
> localH2O = h2o.init(nthreads = -1)
```

The function `h2o.init()` will initialize a H2O instance and instantiates a H2O client module. By default, the H2O instance will launch on `localhost:54321`. To establish a connection to an existing H2O cluster node, explicitly state the IP address (`ip = "localhost"`) and port number (`port = 54321`) in the `h2o.init()` call.

Run the following command to observe an example classification model built through H2O's GLM:

```
# Build a GLM model on prostate data with formula: CAPSULE ~ AGE + RACE
    + PSA + DCAPS
> prostatePath = system.file("extdata", "prostate.csv", package = "h2o")
> prostate.hex = h2o.importFile(localH2O, path = prostatePath, key = "
    prostate.hex")
> h2o.glm(y = "CAPSULE", x = c("AGE","RACE","PSA","DCAPS"), data =
    prostate.hex, family = "binomial", nfolds = 0, alpha = 0.5,
    lambda_search = FALSE,
use_all_factor_levels = FALSE, variable_importances = FALSE,
    higher_accuracy = FALSE)
```

The output of the model build will include coefficients, as well as some validation statistics:

```
IP Address: 127.0.0.1
Port      : 54321
Parsed Data Key: prostate.hex

GLM2 Model Key: GLMModel__827586bb2c59ba79dc129b8500174940

Coefficients:
      AGE       RACE      DCAPS        PSA  Intercept
 -0.01104   -0.63136    1.31888    0.04713   -1.10896

Normalized Coefficients:
      AGE       RACE      DCAPS        PSA  Intercept
 -0.07208   -0.19495    0.40972    0.94253   -0.33707

Degrees of Freedom: 379 Total (i.e. Null);  375 Residual
Null Deviance:     512.3
Residual Deviance: 449.5  AIC: 459.5
Deviance Explained: 0.12254
 Best Threshold: 0.28

Confusion Matrix:
        Predicted
Actual   false true Error
  false     75  152 0.670
  true      18  135 0.118
  Totals    93  287 0.447

AUC =  0.7157151 (on train)
```

4.1 Support

Users of the H2O package may submit general enquiries and bug reports to H2O.ai support address, h2ostream@googlegroups.com. Alternatively, specific bugs or issues may be filed to the H2O.ai JIRA at https://0xdata.atlassian.net/secure/Dashboard.jspa.

5 Generalized Linear Modeling

This section contains a brief overview of generalized linear models and follows up with a few details for each model family.

Generalized linear models are generalizations of linear regression models. Linear regression models the dependency of response y on a vector of predictors x ($y \sim x^T\beta + \beta_0$). The models are built with the assumptions that y has a gaussian distribution with a variance of σ^2 and the mean is a linear function of x with an offset of some constant β_0, i.e. $y = \mathcal{N}(x^T\beta + \beta_0, \sigma^2)$. These assumptions can be overly restrictive for real-world data that do not necessarily have a gaussian distribution. GLM generalizes linear regression in the following ways:

- adding a non-linear link function that transforms the expectation of response variable, so that $link(y) \sim x^T\beta + \beta_0$.

- allowing variance to depend on the predicted value by specifying the conditional distribution of the response variable or the family argument.

This generalization allows us to use GLM on problems such as binary classification (also known as logistic regression).

5.1 Model Fitting

GLM models are fitted by maximizing the likelihood. For the gaussian family, maximum likelihood is simply the minimal mean squared error, which has an analytical solution and can be solved with ordinary least squares. For all other families, the maximum likelihood problem has no analytical solution so we must use an iterative method such as IRLSM, Newton method, gradient descent, or L-BFGS.

5.2 Model Validation

Evaluating the quality of the model is a critical part of any data-modeling and scoring process. There are several standard ways to evaluate the quality of the fitted GLM model; the most common method is to use the resulting deviance. Deviance is calculated by comparing the log likelihood of the fitted model with log likelihood of the saturated model (or theoretically perfect model).

$$deviance = 2(ln(L_s) - ln(L_m))$$

Another metric frequently used for model selection is the Akaike information criterion (AIC). The AIC measures the relative quality of a statistical model for a given set of data obtained by calculating the information loss after replacing the original data with the model itself. Unlike deviance, which would assign a perfect value for the saturated model and measures the absolute quality of the fit with a comparison against the null-hypothesis, AIC takes into account the complexity of the given model. AIC is defined as follows:

$$aic = 2(k - ln(L_m))$$

where k is the number of model parameters and $ln(L_m)$ is the log likelihood of the fitted model over the data.

5.3 Regularization

We introduce penalties to the model building process to avoid over-fitting, reduce variance of the prediction error, and handle correlated predictors. There are two common penalized linear models: ridge regression and lasso. Ridge regression provides greater numerical stability and is easier and faster to compute. In comparison, lasso leads to a sparse solution, which is advantageous in many situations, as it can be used for feature selection and to produce models with fewer parameters. When encountering highly correlated columns, the L2 penalty tends to push all of the coefficients towards each other, while the L1 penalty will pick one and remove the others to produce 0 coefficients.

5.3.1 Lasso

Lasso represents the L1 penalty and is an alternative regularized least squares method that uses the constraint $||B||_1$. The penalty is configured using the `alpha` parameter. The main difference between lasso and ridge regression is that as the penalty for ridge regression increases, the parameters are reduced to non-zero values.

With lasso, if the penalty is increased, the parameters can be reduced to zero values. Since reducing parameters to zero removes them from the model, the lasso method provides only the relevant data. Ridge regression never removes any data.

5.3.2 Elastic Net Penalty

H2O supports elastic net regularization which is parametrized by `alpha` and `lambda` arguments (similar to Regularization Paths for Generalized Linear Models via Coordinate Descent by Friedman et. al)

The `alpha` argument controls the elastic net penalty distribution to L1 and L2 norms. It can have any value in the [0,1] range (inclusive) or a vector of values (triggers grid search). If `alpha = 0`, the result is **Ridge Regression**, while if `alpha = 1` the result is **LASSO**.

The `lambda` argument controls the penalty strength; the range is any positive value or a vector of values (which triggers grid search).

Note: Lambda values are capped at λ_{max}, which is the smallest λ s.t. the solution is empty model (all zeros except for intercept).

Elastic net combines the two and adds another parameter, α, which controls the distribution of the penalty between L1 and L2. The combination of the two penalties is beneficial, since L1 gives sparsity while L2 gives stability and encourages the grouping effect (where a group of correlated variables tends to be dropped or added into the model all at once). One possible use of the α argument is for lasso with very little L2 penalty (α almost 1) to stabilize the computation and improve convergence speed.

A model-fitting problem with an elastic net penalty becomes:

$$\min_{\beta,\beta_0} \frac{1}{N} ln(L(family, \beta, \beta_0)) + \lambda(\alpha\|\beta\|_1 + \frac{1-\alpha}{2}\|\beta\|_2^2)$$

5.4 GLM Models

The following subsection describes the GLM families supported in H2O.

5.4.1 Linear Regression (Gaussian family)

Linear regression refers to the gaussian family model. It is the simplest example of GLM, but it has many uses and several advantages over the other families, such as faster and more stable computation.

It models the dependency as a purely linear function (with link = identity):

$$\hat{y} = x^T\beta + \beta_0$$

The model is fitted by solving the least squares problem (maximum likelihood for gaussian family):

$$\min_{\beta,\beta_0} \frac{1}{2N} \sum_{i=1}^{N} (x_i^T\beta + \beta_0 - y_i)^T(x_i^T\beta + \beta_0 - y_i) + \lambda(\alpha\|\beta\|_1 + \frac{1-\alpha}{2})\|\beta\|_2^2$$

Deviance is simply the sum of squared errors:

$$D = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

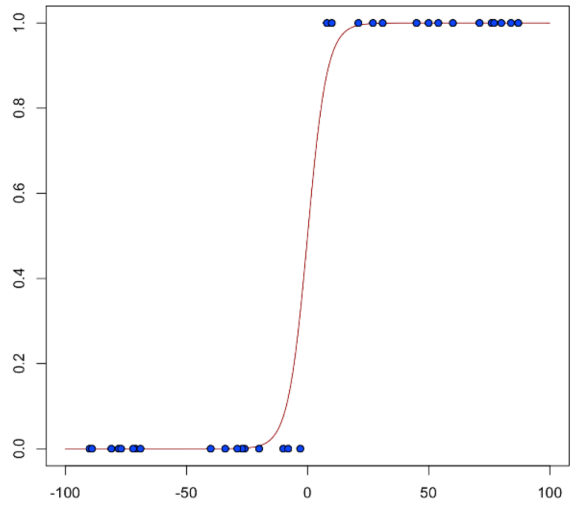
Example

Included in the H2O package is a prostate cancer data set. The data was collected by Dr. Donn Young at Ohio State University Comprehensive Cancer Center for a study of patients with varying degrees of prostate cancer. The following example illustrates how to build a model to predict the volume (VOL) of tumors obtained from ultrasounds based on features such as age and race.

```
> filepath = system.file("extdata", "prostate.csv",package = "h2o")
> prostate.hex = h2o.importFile(object = localH2O, filepath, key = "
    prostate.hex")
> gaussian.fit = h2o.glm(x = c("AGE", "RACE", "PSA", "GLEASON"), y = "
    VOL", data = prostate.hex, family = "gaussian")
```

5.4.2 Logistic Regression (Binomial Family)

Logistic regression can be used for a binary classification problem where the response is categorical with two levels. It models dependency as $Pr(y = 1|x)$. The canonical link for binomial family is logit (log of the odds) and its inverse is a logistic function that takes any real number on the input and projects it onto the 0,1 range (s-curve). The s-curve is shown below:



$$\hat{y} = Pr(y = 1|x) = \frac{e^{x^T\beta+\beta_0}}{1 + e^{x^T\beta+\beta_0}}$$

or alternatively:

$$log\frac{\hat{y}}{1-\hat{y}} = log\frac{Pr(y = 1|x)}{Pr(y = 0|x)} = x^T\beta + \beta_0$$

The model is fitted by solving:

$$\min_{\beta,\beta_0} \frac{1}{N}\sum_{i=1}^{N}(y_i(x_i^T\beta + \beta_0) - log(1 + e^{x_i^T\beta+\beta_0}) + \lambda(\alpha\|\beta\|_1 + \frac{1-\alpha}{2})\|\beta\|_2^2$$

Deviance is -2 log likelihood:

$$D = -2\sum_{i=1}^{N}(ylog(\hat{y}) + (1-y)log(1-\hat{y}))$$

Example

Using the prostate data set, build a binomial model that classifies if there is penetration of the prostatic capsule (CAPSULE). Make sure the entries in the CAPSULE column are binary entries by using the `h2o.table()` function. Change the regression by setting the family to binomial.

```
> h2o.table(prostate.hex[,"CAPSULE"])
  row.names Count
1         0   227
2         1   153
> binomial.fit = h2o.glm(x = c("AGE", "RACE", "PSA", "GLEASON"), y = "
   CAPSULE", data = prostate.hex, family = "binomial")
```

5.4.3 Poisson Models

Poisson regression is generally used in cases where the response represents counts and we assume errors have a Poisson distribution. In general, it can be applied to any data where the response is non-negative.

When building a Poisson model, we usually model dependency of the mean on the log scale, i.e. canonical link is log and prediction is:

$$\hat{y} = e^{x^T\beta+\beta_0}$$

The model is fitted by solving:

$$\min_{\beta,\beta_0}\frac{1}{N}\sum_{i=1}^{N}(y_i(x_i^T\beta+\beta_0) - e^{x_i^T\beta+\beta_0}) + \lambda(\alpha\|\beta\|_1 + \frac{1-\alpha}{2})\|\beta\|_2^2$$

Deviance is

$$D = -2\sum_{i=1}^{N}(ylog(\hat{y}) - y - \hat{y}$$

Example

Load the Insurance data from the MASS library and import into H2O. Run a poisson model that predicts the number of claims (Claims) based on the district of the policy holder (District), their age (Age), and the type of car they own (Group).

```
> library(MASS)
> data(Insurance)
> insurance.hex = as.h2o(localH2O, Insurance)
> poisson.fit = h2o.glm(x = c("District", "Group", "Age"), y = "Claims",
    data = insurance.hex, family = "poisson")
```

5.4.4 Gamma Models

The gamma distribution is useful for modeling a positive continuous response variable, where the conditional variance of the response grows with its mean but the coefficient of variation of the response $\sigma^2(x)/(x)$ is constant for all x, i.e., it has a constant coefficient of variation.

It is usually used with inverse or log link, inverse is the canonical link.

The model is fitted by solving:

$$\min_{\beta,\beta_0} \frac{1}{N} \sum_{i=1}^{N} \frac{y_i}{(x_i^T \beta + \beta_0)} - log(x_i^T \beta + \beta_0) + \lambda(\alpha \|\beta\|_1 + \frac{1-\alpha}{2}) \|\beta\|_2^2$$

Deviance is

$$D = -2 \sum_{i=1}^{N} log(\frac{y_i}{\hat{y}_i}) - \frac{y_i - \hat{y}_i}{\hat{y}_i}$$

Example

To change the link function from the default inverse function to the log link function, modify the `link` argument.

```
> gamma.inverse <- h2o.glm(x=c("AGE","RACE","CAPSULE","DCAPS","PSA","VOL
    "), y="DPROS", data=prostate.hex, family="gamma", link="inverse")

> gamma.log <- h2o.glm(x=c("AGE","RACE","CAPSULE","DCAPS","PSA","VOL"),
    y="DPROS", data=prostate.hex, family="gamma", link="log")
```

6 GLM on H2O

H2O's GLM implementation presents a high-performance distributed algorithm, which scales linearly with the number of rows and works extremely well for datasets with limited number of active predictors.

6.1 Input Parameters

This section describes the specifics of GLM implementation on H2O, such as selecting regularization parameters and handling of categoricals.

6.1.1 Predictors & Response

Every model must specify its predictors and response; it is the equivalent formula object in R. Predictors and response are specified by `source`, `x`, and `y` parameters, with an optional `offset` parameter.

`source` refers to a frame containing a training dataset. All predictors and the response (and offset, if there is one) must be part of this frame.

`x` contains the list of column names or column indices referring to vectors from the source frame; it can not contain periods.

`y` is a column name or index referring to a vector from the source frame.

`offset` is a column name or index referring to a vector from the source frame.

6.1.2 Family & Link

Family and Link are both optional parameters. The default family is `Gaussian` and the default link is a canonical link for the selected family. These are passed in as strings, e.g. `family='gamma', link = 'log'`. While it is possible to select something other than a canonical link, doing so can lead to an unstable computation. Recommended combinations are:

- `Gaussian` and `Log`
- `Inverse, Gamma,` and `Log`

6.1.3 Lambda-Search

Lambda search is a special case of automatic and efficient grid search over lambda argument and is described in its own section. Lambda search can be enabled by using the `lambda_search = T` option. It can be further parametrized by the `nlambdas` and `lambda_min_ratio` parameters. `nlambdas` specifies the number of lambda values on the regularization path and `lambda_min_ratio` specifies the minimal lambda value to be computed as a ration of λ_{max}.

6.2 Coefficient Constraints

Coefficient constraints allow you to set special conditions over the model coefficients. Currently supported constraints are upper and lower bounds and the proximal operator interface, as described in Proximal Algorithms by Boyd et. al.

The constraints are specified as a frame with following vecs (matched by name; all vecs can be sparse):

- `names (mandatory)` - coefficient names.
- `lower_bounds (optional)` - coefficient lower bounds , must be $<= 0$
- `upper_bounds (optional)` - coefficient upper bounds , must be $>= 0$
- `beta_given (optional)` - specifies the given solution in proximal operator interface
- `rho` (mandatory if `beta_given` is specified, otherwise ignored) - specifies per-column L2 penalties on the distance from the given solution

The proximal operator interface allows you to run the GLM with a proximal penalty on a distance from a specified given solution. There are many potential uses: for example, it can be used as part of an ADMM consensus algorithm to obtain a unified solution over separate H2O clouds, or in Bayesian regression approximation.

6.3 H2O GLM Model Output

The detailed output of the GLM model varies depending on the distribution used for the model. In general, there is shared output for all Families: Coefficients & Normalized Coefficients, Validation, and Prediction. We'll cover the model output from an R user's point of view.

First, let's build a simple GLM on a small dataset and see what we get out:

```
library(h2o)

# Initialize H2O
h <- h2o.init()

# path to the data
data.bucket <- "https://raw.githubusercontent.com/h2oai/h2o/master/
   smalldata"
data.path <- paste(data.bucket, "/logreg/prostate_train.csv", sep = "")

# import the data from the url
hex <- h2o.importFile(h, data.path)

# build a binomial regression
m <- h2o.glm(x = 3:9, y = 2, data = hex, family = "binomial")
# no other features tweaked... yet
```

The default show of this model has the following output:

```
IP Address: 127.0.0.1
Port      : 54321
Parsed Data Key: prostate_train.hex

GLM2 Model Key: GLMModel__8b954fd700d924f3e9dee8717b8246ef

Coefficients:
      AGE      RACE     DPROS     DCAPS       PSA       VOL   GLEASON Intercept
 -0.07668  -0.10320   0.59479   0.13549   0.43841  -0.22215   1.19657  -0.49458

Normalized Coefficients:
      AGE      RACE     DPROS     DCAPS       PSA       VOL   GLEASON Intercept
 -0.07668  -0.10320   0.59479   0.13549   0.43841  -0.22215   1.19657  -0.49458

Degrees of Freedom: 304 Total (i.e. Null);  297 Residual
Null Deviance:     412.1
Residual Deviance: 301.9  AIC: 317.9
Deviance Explained: 0.26733
 Best Threshold: 0.44

Confusion Matrix:
        Predicted
Actual   false true Error
  false    147   34 0.188
  true      32   92 0.258
  Totals   179  126 0.216

AUC =  0.8318927 (on train)
```

Briefly, the output contains the IP address and port number of the H2O cluster where the model was trained. It includes the data key, the model key, the coefficients, and some model metrics. Let's look at these in detail.

6.3.1 Coefficients & Normalized Coefficients

Coefficients are the predictor weights (i.e. the actual model used for prediction). If the `standardize` option is enabled, H2O returns another set of coefficients, the normalized coefficients. These are the predictor weights of the standardized data and are included only for informational purposes (e.g. to compare relative variable importance). In this case, the coefficients are obtained from the normalized coefficients by **reversing** the data standardization process (de-scaled, with the intercept adjusted by an added offset) so that they can be applied to data in its original form (i.e. no standardization prior to scoring). **Note:** These are **not** the same as coefficients of a model built on non-standardized data.

6.3.2 Validation

By default, H2O's GLM generates additional models with 1/10 of the original data to performs 10-fold cross-validation. This will provide a quick idea of how the model will generalize. However, it's always best to evaluate the model using some holdout data.

6.3.3 Generating Predictions

The following R code generates predictions:

```
test.path <- paste(data.bucket, "/logreg/prostate_test.csv", sep = "")

# import the data from the url
test <- h2o.importFile(h, test.path)

# generate the predictions
predictions <- h2o.predict(m, test)

# look at the first 6 entries of predictions
predictions

# generate the model metrics
h2o.performance(data=predictions[,3], reference=test[,1])
```

6.4 Categorical Variables

When applying linear models to datasets with categorical variables, the usual approach is to expand the categoricals into a set of binary vectors, with one vector per each categorical level (e.g. by calling `model.matrix` in R). H2O performs similar expansions automatically and no prior changes to the dataset are needed. Each categorical column is treated as a set of sparse binary vectors.

6.4.1 Largest Categorical Trick

Categoricals have special handling during GLM computation as well. When forming the gram matrix, we can take advantage of the fact that columns belonging to the same categorical never co-occur and the gram matrix region belonging to these columns will not have any non-zero elements outside of the diagonal. We can thus keep it in sparse representation, taking only O(N) elements instead of O(N*N). Furthermore, the complexity of Choelsky decomposition of a matrix that starts with a diagonal region can be greatly reduced. H2O's GLM exploits these two facts to handle the largest categorical "for free". Therefore, when analyzing the performance

of GLM in the equation expressed above, we can subtract the size of the largest categoricals from the number of predictors.

$$N = \sum_{c \in C} (\|c.domain\|) - \arg\max_{c \in C} \|c.domain\| + \|Nums\|$$

6.5 Cross-Validation

All validation values can be computed using either the training data set (the default option) or using N-fold cross-validation (`nfolds` > 1). When N-fold cross-validation is enabled, H2O randomly splits data into n equally-sized parts, trains each of the n models on n-1 parts, and computes validation on the part that was not used for training. The reported validation parameters are then obtained as follows:

- Null deviance is sum of null deviances of n-models (each uses null model based on the subset of the data)
- Residual deviance is sum of residual deviances of all n-models
- AIC is based on log-likelihood, which is summed up similarly to deviance
- AUC is based on ROC curve build by summing up confusion matrices built for all n-models. For each threshold, we get a confusion matrix that includes all the rows from the training set. However, each row is classified exclusively by the model that did not contain that row in its training set. The computation of AUC is the same as for a model without cross-validation.

6.6 Selecting Regularization Parameters

To get the best possible model, we need to find the optimal values of the regularization parameters α and λ. To find the optimal values, H2O provides grid search over α and a special form of grid search called "lambda search over λ". The recommended way to find optimal regularization settings on H2O is to do a grid search over a few α values with an automatic lambda search for each α. Both are described below in greater detail.

6.6.1 Grid Search Over Alpha

Alpha search is not always needed and simply changing its value to 0.5 (or 0 or 1 if we only want Ridge or Lasso, respectively) works in most cases. If α search is needed, usually only a few values are sufficient. Alpha search is invoked by supplying a list of values for α instead of a single value. H2O then produces one model per α value. The grid search computation can be done in parallel (depending on the cluster resources) and it is generally more efficient than computing different models separately from R.

Use caution when including $\alpha = 0$ or $\alpha = 1$ in the grid search. $\alpha = 0$ will produce a dense solution and it can be really slow (or even impossible) to compute in large N situations. $\alpha = 1$ has no L2 penalty, so it is therefore less numerically stable and can be very slow as well due to slower convergence. In general, it is safer to run with $alpha = 1 - \epsilon$ instead.

6.6.2 Lambda Search

Lambda search can be enabled by using the `lambda_search = T` option. It can be further parametrized by the `nlambdas` and `lambda_min_ratio` parameters. When this option is enabled, H2O performs a specialized grid search over the list of `nlambdas` λ values, producing one model for each λ value.

The λ-list is automatically generated as an exponentially decreasing sequence, going from λ_{max}, the smallest λ s.t. the solution is a model with all 0s, to λ_{min} = *lambda_min_ratio* * λ_{max}.

H2O computes λ-models sequentially and in decreasing order, warm-starting (using the previous solution as the initial prediction) the model for λ_k with the solution for λ_{k-1}. By warm-starting the models, we get better performance: typically models for subsequent λs are close to each other, so we need only a few iterations per λ (typically 2 or 3). We also achieve greater numerical stability, since models with a higher penalty are easier to compute, so we start with an easy problem and then keep making only small changes to it.

Note: `nlambda` and `lambda_min_ratio` also specify the relative distance of any two lambdas in the sequence. This is important when applying recursive strong rules, which are only effective if the neighboring lambdas are "close" to each other. The default values are `nlambda` = 100 and $\lambda_{min} = \lambda_{max} 1e^{-4}$, which gives us the ratio of 0.912. For best results when using strong rules, keep the ratio close to the default.

6.6.3 Grid Search Over Lambdas

While automatic lambda search is the preferred method, it is also possible to do a grid search over lambda values by passing in vector of lambdas and disabling the lambda-search option. The behavior will be identical to lambda search, except H2O will use a user-supplied list of lambdas instead (still capped at λ_{max}).

6.7 Strong Rules

H2O's GLM employs strong rules (as described in Strong Rules for Discarding Predictors in Lasso-type Problems by Bien et. al) to discard predictors that are likely to have 0 coefficients prior to model building. According to Strong Rules for Discarding Predictors in Lasso-type Problems by Bien et. al, we can identify these predictors based on a gradient with great accuracy. This provides very few false negatives and virtually no false positives in practice, greatly reducing the computational complexity of model fitting and enabling it to run on wide datasets with tens of thousands of predictors, provided that there is a limited number of active predictors.

When applying the strong rules, we evaluate the gradient at the starting solution, filter out inactive coefficients, and fit a model using only a subset of the available predictors. Since strong rules may have false positives (which are extremely rare in practice), we need to check the solution by testing the kkt conditions and verify that all discarded predictors indeed have 0 coefficients.

6.8 Performance Characteristics

The implementation is based on iterative re-weighted least squares with an ADMM inner solver (as described in Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers by Boyd et. al) to deal with the L1 penalty. Every iteration of the algorithm consists of following steps:

1. Generate weighted least squares problem based on previous solution, i.e. vector of weights w and response z
2. Compute the weighted gram matrix $X^T W X$ and $X^T z$ vector
3. Decompose the gram matrix (Cholesky decomposition) and apply ADMM solver to solve the L1 penalized least squares problem

Steps 1 and 2 are performed distributively and step 3 is computed in parallel on a single node. We can thus characterize the computational complexity and scalability of dataset with M observations and N columns (predictors) on a cluster with n nodes with p CPUs each as follows:

$$O(\frac{MN^2}{pn} + \frac{N^3}{p})$$

And the overall memory cost is given by:

$$O(MN + N^2pn)$$

If $M >> N$, the second term is not needed and the algorithm scales linearly both in the number of nodes and the number of CPUs per node. However, the equation above also implies that our algorithm is limited in the number of predictors it can handle, since the size of the Gram matrix grows quadratically due to a memory and network throughput issue with the number of predictors and its decomposition cost grows as the cube of the number of predictors (which is a computational cost issue). In many cases, H2O can work around these limitations due to its handling of categoricals and by employing strong rules to filter out inactive predictors.

7 Use case: Classification with Airline data

7.1 Airline dataset overview

Download the Airline dataset here:
https://github.com/h2oai/h2o/blob/master/smalldata/airlines/allyears2k_headers.zip.

Save the .csv file to your working directory by clicking "View Raw." Before running the Airline demo, we'll review how to load data with H2O.

7.1.1 Loading data

Loading a dataset in R for use with H2O is slightly different from the usual methodology because we must convert our datasets into `H2OParsedData` objects. In this example, we will use a toy weather dataset that is available here:
https://raw.githubusercontent.com/h2oai/h2o/master/smalldata/weather.csv.

First, load the data to your current working directory in your R Console (do this for any future dataset downloads), and then run the following command:

```
weather.hex = h2o.uploadFile(localH2O, path = "weather.csv", header =
    TRUE, sep = ",", key = "weather.hex")
```

To see a quick summary of the data, run the following command:

```
summary(weather.hex)
```

7.2 Performing a trial run

Returning to the Airline dataset demo, we first load the dataset into H2O and select the variables we want to use to predict a chosen response. For example, we can model if flights are delayed based on the departure's scheduled day of the week and day of the month.

```
library(h2o)
localH2O = h2o.init(nthreads = -1)
#Load the data and prepare for modeling
air_train.hex = h2o.uploadFile(localH2O, path = "~/Downloads/
   AirlinesTrain.csv", header = TRUE, sep = ",", key = "airline_train.
   hex")
air_test.hex = h2o.uploadFile(localH2O, path = "~/Downloads/AirlinesTest
   .csv", header = TRUE, sep = ",", key = "airline_test.hex")
x = c("fYear", "fMonth", "fDayofMonth", "fDayOfWeek", "UniqueCarrier", "
   Origin", "Dest", "Distance")
y = "IsDepDelayed"
```

Now we train the GLM model:

```
airline.glm <- h2o.glm(x=x,
                       y=y,
                       data=air_train.hex,
                       key = "glm_model",
                       family="binomial",
                       lambda_search = TRUE,
                       return_all_lambda = TRUE,
                       use_all_factor_levels = TRUE,
                       variable_importances = TRUE)
```

7.2.1 Extracting and handling the results

We can extract the parameters of our model, examine the scoring process, and make predictions on new data.

```
print("Predict on GLM model")
best_glm = airline.glm@models[[airline.glm@best_model]]
air.results = h2o.predict(object = best_glm, newdata = air_test.hex)
print("Check performance and AUC")
perf = h2o.performance(air.results$YES,air_test.hex$IsDepDelayed )
print(perf)
perf@model$auc
print("Show distribution of predictions with quantile.")
quant = quantile.H2OParsedData(air.results$YES)
print("Extract strongest predictions.")
top.air <- h2o.assign(air.results[air.results$YES > quant["75%"]], key="
   top.air")
top.air
```

Once we have a satisfactory model, the `h2o.predict()` command can be used to compute and store predictions on the new data, which can then be used for further tasks in the interactive modeling process.

```
#Perform classification on the held out data
prediction = h2o.predict(object = best_glm, newdata=air_test.hex)
#Copy predictions from H2O to R
pred = as.data.frame(prediction)
head(pred)
```

7.3 Web interface

H2O R users have access to an intuitive web interface for H2O, Flow, to mirror the model building process in R. After loading data or training a model in R, point your browser to your IP address and port number (e.g., localhost:12345) to launch the web interface. From here, you can click on ADMIN > JOBS to view specific details about your model. You can also click on DATA > LIST ALL FRAMES to view all current H2O frames.

7.3.1 Variable importances

The variable importances feature can be enabled with the argument `variable_importances=TRUE`.This feature allows us to view the absolute and relative predictive strength of each feature in the prediction task. From R, you can access these strengths with the command `air.model@model$varimp`. You can also view a visualization of the variable importances on the web interface.

7.3.2 Java model

Java models are currently not available for GLM. To download the model,

1. Open the terminal window.
2. Create a directory where the model will be saved.
3. Set the new directory as the working directory.
4. Follow the curl and java compile commands displayed in the instructions at the top of the Java model.

8 Appendix: Parameters

- `x`: A vector containing the names of the predictors to use while building the GLM model. No default.
- `y`: A character string or index that represents the response variable in the model. No default.
- `training_frame`: An `H2OFrame` object containing the variables in the model.
- `model_id`: (Optional) The unique ID assigned to the generated model. If not specified, an ID is generated automatically.
- `validation_frame`: An `H2OParsedData` object containing the validation dataset used to construct confusion matrix. If blank, the training data is used by default.
- `max_iterations`: A non-negative integer specifying the maximum number of iterations.
- `beta_epsilon`: A non-negative number specifying the magnitude of the maximum difference between the coefficient estimates from successive iterations. Defines the convergence criterion.
- `solver`: A character string specifying the solver used: either `IRLSM`, which supports more features, or `L_BFGS`, which scales better for datasets with many columns.
- `standardize`: A logical value that indicates whether the numeric predictors should be standardized to have a mean of 0 and a variance of 1 prior to model training.
- `family`: A description of the error distribution and corresponding link function to be used in the model. The following options are supported: `gaussian`, `binomial`, `poisson`, `gamma`, or `tweedie`. When a model is specified as Tweedie, users must also specify the appropriate Tweedie power. No default.
- `link`: The link function relates the linear predictor to the distribution function. The default is the canonical link for the specified family. The full list of supported links:
  - **gaussian**: identity, log, inverse
  - **binomial**: logit, log
  - **poisson**: log, identity
  - **gamma**: inverse, log, identity
  - **tweedie**: tweedie
- `tweedie_variance_power`: A numeric specifying the power for the variance function when `family = "tweedie"`.
- `tweedie_link_power`: A numeric specifying the power for the link function when `family = "tweedie"`.
- `alpha`: The elastic-net mixing parameter, which must be in $[0, 1]$. The penalty is defined to be $P(\alpha, \beta) = (1 - \alpha)/2||\beta||_2^2 + \alpha||\beta||_1 = \sum_j [(1 - \alpha)/2\beta_j^2 + \alpha|\beta_j|]$ so `alpha=1` is the lasso penalty, while `alpha=0` is the ridge penalty. Default is 0.5.
- `prior`: (Optional) A numeric specifying the prior probability of class 1 in the response when `family = "binomial"`. The default value is the observation frequency of class 1.
- `lambda`: A non-negative value representing the shrinkage parameter, which multiplies $P(\alpha, \beta)$ in the objective. The larger lambda is, the more the coefficients are shrunk toward zero (and each other). When the value is 0, no elastic-net penalty is applied and ordinary generalized linear models are fit. Default is 1e-5.
- `lambda_search`: A logical value indicating whether to conduct a search over the space of lambda values, starting from the max lambda, given lambda will be interpreted as the min. lambda. Default is false.

- nlambdas: The number of lambda values when lambda_search = TRUE. Default is -1.
- lambda_min_ratio: Smallest value for lambda as a fraction of lambda.max, the entry value, which is the smallest value for which all coefficients in the model are zero. If the number of observations is greater than the number of variables then lambda_min_ratio = 0.0001; if the number of observations is less than the number of variables then lambda_min_ratio = 0.01. Default is -1.
- nfolds: Number of folds for cross-validation. If nfolds >=2, then validation_frame must remain blank. Default is 0.
- fold_column: (Optional) Column with cross-validation fold index assignment per observation.
- fold_assignment: Cross-validation fold assignment scheme, if fold_column is not specified. The following options are supported: AUTO, Random, or Modulo.
- keep_cross_validation_predictions: Specify whether to keep the predictions of the cross-validation models.
- beta_constraints: A data frame or H2OParsedData object with the columns ["names", "lower_bounds", "upper_bounds", "beta_given"], where each row corresponds to a predictor in the GLM. "names" contains the predictor names, "lower_bounds"/"upper_bounds" are the lower and upper bounds (respectively) of the beta, and "beta_given" is a user-specified starting value.
- offset_column: Specify the offset column. Note: Offsets are per-row bias values that are used during model training. For Gaussian distributions, they can be seen as simple corrections to the response (y) column. Instead of learning to predict the response (y-row), the model learns to predict the (row) offset of the response column. For other distributions, the offset corrections are applied in the linearized space before applying the inverse link function to get the actual response values.
- weights_column: Specify the weights column. Note: Weights are per-row observation weights. This is typically the number of times a row is repeated, but non-integer values are supported as well. During training, rows with higher weights matter more, due to the larger loss function pre-factor.
- intercept: Logical; includes a constant term (intercept) in the model. If there are factor columns in your model, then the intercept must be included.

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