

Generalized Linear Modeling with H2O

TOMAS NYKODYM

ARIEL RAO

AMY WANG

TOM KRALJEVIC

JESSICA LANFORD

<http://h2o.gitbooks.io/glm-with-h2o/>

August 2015: Third Edition

Generalized Linear Modeling with H2O

by Tomas Nykodym, Ariel Rao, Amy Wang, Tom Kraljevic, & Jessica Lanford

Published by H2O.ai, Inc.

2307 Leghorn St.

Mountain View, CA 94043

©2015 H2O.ai, Inc. All Rights Reserved.

August 2015: Third Edition

Photos by ©H2O.ai, Inc.

While every precaution has been taken in the preparation of this book, the publisher and authors assume no responsibility for errors or omissions, or for damages resulting from the use of the information contained herein.

Printed in the United States of America.

Contents

1	Introduction	3
2	What is H2O?	3
3	Installation	4
3.1	Installation in R	4
3.2	Installation in Python	4
3.3	Pointing to a different H2O cluster	5
3.4	Example code	5
4	GLM Concepts	6
4.1	GLM in H2O	6
4.2	Model fitting	7
4.3	Model validation	7
4.4	Regularization	8
4.4.1	Lasso and Ridge regression	8
4.4.2	Elastic net penalty	8
4.5	GLM model families	9
4.5.1	Linear regression (Gaussian family)	9
4.5.2	Logistic regression (Binomial family)	10
4.5.3	Poisson models	11
4.5.4	Gamma models	12
4.5.5	Tweedie models	14
5	Building GLM Models in H2O	14
5.1	Classification vs. regression	14
5.2	Training and validation frames	15
5.3	Predictor and response variables	15
5.3.1	Categorical variables	16
5.4	Family and link	16
5.5	Regularization parameters	16
5.5.1	alpha and lambda	16
5.5.2	Lambda Search	17
5.6	Handling wide data and building sparse models	18
5.6.1	Solver selection	18
5.6.2	Stopping criteria	18
5.7	Advanced features	19
5.7.1	Standardizing data	19
5.7.2	N-fold cross validation	19
5.7.3	Grid search over alpha	20
5.7.4	Grid search over lambda	21
5.7.5	Offsets	21
5.7.6	Row weights	21
5.7.7	Coefficient constraints	21

5.7.8 Proximal operators	22
6 GLM Model Output	22
6.1 Coefficients and normalized coefficients	24
6.2 Model statistics	25
6.3 Confusion matrix	26
6.4 Scoring history	26
7 Making Predictions	26
7.1 Batch in-H2O predictions	26
7.2 Low-latency predictions with the NanoFast scoring engine	28
8 Best Practices	28
8.1 Verifying Model Results	29
9 Implementation Details	30
9.1 Categorical variables	30
9.1.1 Largest categorical speed optimization	30
9.2 Speed and memory performance characteristics	31
9.2.1 IRLSM solver	31
9.2.2 L-BFGS solver	32
9.3 Data corner cases	32
10 H2O Community Resources	32
11 Appendix: Parameters	32

1 Introduction

This document introduces the reader to Generalized Linear Modeling with H2O. Examples are written in R and python. The reader is walked through the installation of H2O, basic GLM concepts, building GLM models in H2O, how to interpret model output, how to make predictions, and various implementation details.

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 their data without sampling to get accurate predictions faster. Advanced algorithms, like Deep Learning, Boosting, and Bagging Ensembles are built-in to help application designers create smarter applications through elegant APIs. Some of our initial 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 industries.

Using in-memory compression, H2O handles billions of data rows in-memory, even with a small cluster. To make it easier for non-engineers to create complete analytic workflows, H2O's platform includes interfaces for R, Python, Scala, Java, JSON, and Coffeescript/JavaScript, as well as a built-in web interface, Flow. H2O was built alongside (and on top of) Hadoop and Spark Clusters and typically deploys within minutes.

H2O includes many 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 at scale, such as Random Forest, Gradient Boosting and Deep Learning. Customers can build thousands of models and compare the results to get the best predictions.

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

Try it out

H2O's R package can be installed from CRAN at <https://cran.r-project.org/web/packages/h2o/>. A Python package can be installed from PyPI at <https://pypi.python.org/pypi/h2o/>. Download H2O directly from <http://h2o.ai/download>.

Join the community

Visit the open source community forum at <https://groups.google.com/d/forum/h2ostream>. To learn about our meetups, training sessions, hackathons, and product updates, visit <http://h2o.ai>.

3 Installation

The easiest way to directly install H2O is via an R or Python package.

(**Note:** This document was created with H2O version 3.0.1.4.)

3.1 Installation in R

To load a recent H2O package from CRAN, run:

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

(**Note:** The version of H2O in CRAN is often one release behind the current version.)

Alternatively, you can (and should for this tutorial) download the latest stable H2O-3 build from the H2O download page:

1. Go to <http://h2o.ai/download>.
2. Choose the latest stable H2O-3 build.
3. Click the "Install in R" tab.
4. Copy and paste the commands into your R session.

After H2O is installed on your system, verify the installation:

```
1 library(h2o)
2
3 # Start H2O on your local machine using all available cores.
4 # By default, CRAN policies limit use to only 2 cores.
5 h2o.init(nthreads = -1)
6
7 # Get help
8 ?h2o.glm
9 ?h2o.gbm
10
11 # Show a demo
12 demo(h2o.glm)
13 demo(h2o.gbm))
```

3.2 Installation in Python

To load a recent H2O package from PyPI, run:

```
1 pip install h2o
```

Alternatively, you can (and should for this tutorial) download the latest stable H2O-3 build from the H2O download page:

1. Go to <http://h2o.ai/download>.
2. Choose the latest stable H2O-3 build.
3. Click the "Install in Python" tab.
4. Copy and paste the commands into your Python session.

After H2O is installed, verify the installation:

```
1 import h2o
2
3 # Start H2O on your local machine
4 h2o.init()
5
6 # Get help
7 help(h2o.glm)
8 help(h2o.gbm)
9
10 # Show a demo
11 h2o.demo("glm")
12 h2o.demo("gbm")
```

3.3 Pointing to a different H2O cluster

Following the instructions in the previous sections create a one-node H2O cluster on your local machine.

To connect to an established H2O cluster (in a multi-node Hadoop environment, for example) specify the IP address and port number for the established cluster using the `ip` and `port` parameters in the `h2o.init()` command:

```
1 h2o.init(ip="123.45.67.89", port=54321)
```

3.4 Example code

R code for the examples in this document are available here:

https://github.com/h2oai/h2o-3/blob/master/h2o-docs/src/booklets/v2_2015/source/GLM_Vignette.R

Python code for the examples in this document can be found here:

https://github.com/h2oai/h2o-3/blob/master/h2o-docs/src/booklets/v2_2015/source/GLM_Vignette.py

The document source itself can be found here:

https://github.com/h2oai/h2o-3/blob/master/h2o-docs/src/booklets/v2_2015/source/GLM_Vignette.tex

4 GLM Concepts

Generalized linear models (GLM) are the workhorse for most predictive analysis use cases. GLM scales well to large datasets, is based on a solid statistical background, and can be used for both regression and classification. 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.

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).

4.1 GLM in 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 (\sim 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:

$$\min_{\beta} (ClassicGLM + RegularizationPenalty)$$

which is equivalent to:

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

The elastic net parameter α controls the penalty distribution between L1 (Lasso) and L2 (Ridge Regression) penalties. 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 a null-model (maximum penalty) down to a minimally-penalized model. To improve the efficiency of this search, H2O employs 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 because 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.

4.2 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 a standard method of 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.

4.3 Model validation

Evaluating the quality of the model is a critical part of the 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 the 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.

4.4 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 (least absolute shrinkage and selection operator). 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.

4.4.1 Lasso and Ridge regression

Lasso represents the L1 penalty and is an alternative regularized least squares method that uses the constraint $\|B\|_1$. 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 only relies on the relevant data (discards the noise). Ridge regression never removes any predictors.

4.4.2 Elastic net penalty

H2O supports elastic net regularization, which is a combination of L1 and L2 penalties and 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 (which 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).

The combination of L1 and L2 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:

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

4.5 GLM model families

The following subsection describes the GLM families supported in H2O.

4.5.1 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):

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

Deviance is simply the sum of squared errors:

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

Example in R

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.

```

1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 gaussian.fit = h2o.glm(y = "VOL", x = c("AGE", "RACE", "PSA", "
    GLEASON"), training_frame = h2o_df, family = "gaussian")

```

Example in Python

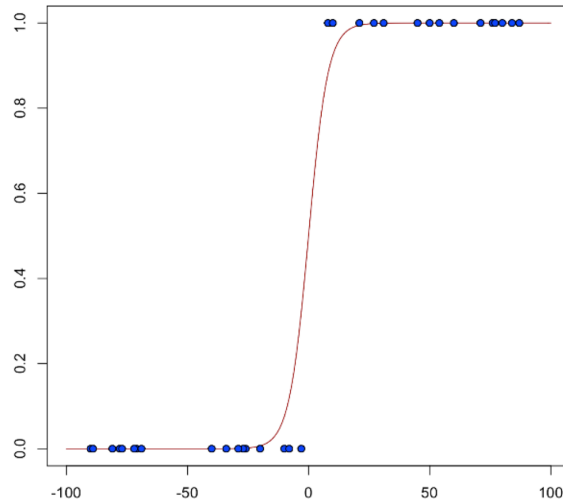
```

1 import h2o
2 h2o.init()
3 path = h2o.system_file("prostate.csv")
4 h2o_df = h2o.import_file(path)
5 gaussian_fit = h2o.glm(y = "VOL", x = ["AGE", "RACE", "PSA", "
    GLEASON"], training_frame = h2o_df, family = "gaussian")

```

4.5.2 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:

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

Deviance is $-2 \log$ likelihood:

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

Example in R

Using the prostate data set, this example builds a binomial model that classifies incidence of penetration of the prostatic capsule (CAPSULE). Confirm the entries in the CAPSULE column are binary using the `h2o.table()` function. Change the regression by changing the family to binomial.

```
1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 is.factor(h2o_df$CAPSULE)
6 h2o_df$CAPSULE = as.factor(h2o_df$CAPSULE)
7 is.factor(h2o_df$CAPSULE)
8 binomial_fit = h2o.glm(y = "CAPSULE", x = c("AGE", "RACE", "PSA",
      "GLEASON"), training_frame = h2o_df, family = "binomial")
```

Example in Python

```
1 import h2o
2 h2o.init()
3 path = h2o.system_file("prostate.csv")
4 h2o_df = h2o.import_file(path)
5 h2o_df['CAPSULE'] = h2o_df['CAPSULE'].asfactor()
6 binomial_fit = h2o.glm(y = "CAPSULE", x = ["AGE", "RACE", "PSA",
      "GLEASON"], training_frame = h2o_df, family = "binomial")
```

4.5.3 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:

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

Example in R

This example loads the Insurance data from the MASS library, imports it into H2O, and runs 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).

```

1 library(h2o)
2 h2o.init()
3 library(MASS)
4 data(Insurance)
5
6 # Convert ordered factors into unordered factors.
7 # H2O only handles unordered factors today.
8 class(Insurance$Group) <- "factor"
9 class(Insurance$Age) <- "factor"
10
11 # Copy the R data.frame to an H2OFrame using as.h2o()
12 h2o_df = as.h2o(Insurance)
13 poisson.fit = h2o.glm(y = "Claims", x = c("District", "Group", "
    Age"), training_frame = h2o_df, family = "poisson")

```

Example in Python

```

1 # No equivalent running example provided for python due to the
2 # license of the MASS R package.
3 #
4 # poisson_fit = h2o.glm(y = "Claims", x = ["District", "Group", "
    Age"], training_frame = h2o_df, family = "poisson")

```

4.5.4 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, where 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:

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

Example in R

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

```
1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 gamma.inverse <- h2o.glm(y = "DPROS", x = c("AGE","RACE","CAPSULE",
6       "DCAPS","PSA","VOL"), training_frame = h2o_df, family = "
       gamma", link = "inverse")
7 gamma.log <- h2o.glm(y="DPROS", x = c("AGE","RACE","CAPSULE","
       DCAPS","PSA","VOL"), training_frame = h2o_df, family = "gamma",
       link = "log")
```

Example in Python

```
1 import h2o
2 h2o.init()
3 path = h2o.system_file("prostate.csv")
4 h2o_df = h2o.import_file(path)
5 gamma_inverse = h2o.glm(y = "DPROS", x = ["AGE","RACE","CAPSULE",
6       "DCAPS","PSA","VOL"], training_frame = h2o_df, family = "gamma"
7       , link = "inverse")
8 gamma_log = h2o.glm(y="DPROS", x = ["AGE","RACE","CAPSULE","DCAPS",
9       "PSA","VOL"], training_frame = h2o_df, family = "gamma", link
10      = "log")
```

4.5.5 Tweedie models

Tweedie models are a class of distributions which include Gamma, Normal, Poisson and their combination. It is especially useful for modelling of variables which have 0s combined with continuous non-zero values (e.g. Gamma distribution).

Tweedie is parametrized by variance power p which can be one of the following:

- 0 Normal
- 1 Poisson
- (1, 2) Compound Poisson, non-negative with mass at zero
- 2 Gamma
- 3 Inverse-Gaussian
- > 2 Stable, with support on the positive reals

TODO fit in likelihood

Deviance for variance p ($p = 1$ and $p = 2$) is :

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

Example in R

```
1 # TODO
```

Example in Python

```
1 # TODO
```

5 Building GLM Models in H2O

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

5.1 Classification vs. regression

GLM can produce two categories of models: classification (binary classification only) and regression. Binary classification in GLM is also called logistic regression.

The data type of the response column determines the model category. If the response data type is a categorical (also called a factor or an enum) then a classification model is created. If the response column data type is numeric (either integer or real), then a regression model is created.

The following examples show how to coerce the data type of a column to a factor.

Example in R

```
1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 h2o_df$CAPSULE = as.factor(h2o_df$CAPSULE)
6 summary(h2o_df)
```

Example in Python

```
1 import h2o
2 h2o.init()
3 path = h2o.system_file("prostate.csv")
4 h2o_df = h2o.import_file(path)
5 h2o_df["CAPSULE"] = h2o_df["CAPSULE"].asfactor()
6 h2o_df.summary()
```

5.2 Training and validation frames

In this context, the word Frame refers to an H2OFrame, which is the fundamental method of data storage in H2O's distributed memory.

`training_frame` refers to a frame containing a training dataset. All predictors and the response (as well as offset and weights, if specified) must be part of this frame.

`validation_frame` refers to an optional frame containing a validation dataset. If specified, this frame must have exactly the same columns as the training dataset. Metrics are calculated on the validation dataset for convenience.

If a validation dataset is not specified during training, there are functions that can calculate the same metrics after the model training is complete.

5.3 Predictor and response variables

Every model must specify its predictors and response. Predictors and response are specified by the `x` and `y` parameters.

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

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

5.3.1 Categorical variables

If the response column is categorical, then a classification model is created. GLM only supports binomial classification, so the response column may only have two levels.

Categorical predictor columns may have more than two levels.

We recommend letting GLM handle categorical columns itself, as it can take advantage of the categorical column for better performance and memory utilization.

We strongly recommend avoidance of one-hot encoding categorical columns with many levels into many binary columns, as this is very inefficient. This is especially true for Python users who are used to expanding their categorical variables manually for other frameworks.

5.4 Family and 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.

5.5 Regularization parameters

Refer to Regularization above for a detailed explanation.

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.

5.5.1 alpha and lambda

`alpha` controls the distribution between L1 (Lasso) and L2 (Ridge regression) penalties. An `alpha` of 1.0 indicates only Lasso, and an `alpha` of 0.0 indicates only ridge.

`lambda` controls the amount of regularization applied. For a `lambda` value of 0.0, no regularization is applied, and the `alpha` parameter is ignored. The default value for `lambda` is calculated by H2O using a heuristic based on the training data. If you let H2O calculate `lambda`, you can see the chosen value in the model output.

5.5.2 Lambda Search

Lambda search enables efficient and automatic search for optimal value of the `lambda` parameter. When lambda search is enabled, GLM will first fit a model with maximum regularization strength and then keep decreasing it until overfitting. The resulting model will be based on the best `lambda` value. When looking for sparse solution (`alpha > 0`), lambda search can also be used to efficiently handle very wide datasets as it can filter out inactive predictors (noise) and only build models for a small subset of predictors. Common use of lambda search is to run on a dataset with many predictors but limit the number of active predictors to relatively small value.

Lambda search can be turned on by setting `lambda_search` and can be further customized by following arguments:

- `alpha` - regularization distribution between L1 and L2
- `validation_frame` and/or `n_folds`: The best `lambda` is selected based on performance on the cross-validation or validation or training data. If available, cross-validation performance takes preference. If no validation data is available, the best `lambda` is selected based on training data performance and is therefore guaranteed to always be the minimal `lambda` computed as GLM can not overfit on a training dataset.

Note: If running lambda search with validation dataset and no cross-validation, validation data set is used to select the `lambda` value, validation dataset is thus contaminated and performance should be evaluated on another independent dataset.

- `lambda_min_ratio` and `nlambdas`:

The sequence of λ -s is automatically generated as an exponentially decreasing sequence, going from λ_{max} , the smallest λ such that the solution is a model with all 0s, to $\lambda_{min} = \text{lambda_min_ratio} * \lambda_{max}$.

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 λ s are close to each other, so we need only a few iterations per λ (typically two or three). 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.

- `max_active_predictors`: Limit the number of active predictors (the actual number of non-zero predictors in the model is going to be slightly lower), useful when obtaining a sparse solution to avoid costly computation of models with too many predictors.

5.6 Handling wide data and building sparse models

H2O's GLM offers two different approaches to handling wide datasets: L1 regularization and the L_BFGS solver.

Quick recommendations:

- For a sparse solution (i.e. some predictors are dropped from the final model), use the IRLSM solver with alpha greater than 0.0 (so you get at least some L1 penalty) and enable `lambda_search`.
- For a dense solution (i.e. all predictors are in the final model), use the L_BFGS solver with alpha of 0 so there is no L1 penalty, only L2 penalty.
- If not sure whether the solution should be sparse or dense, try both cases and pick the better one based on validation (cross-validation) data.

5.6.1 Solver selection

The two solvers provided in H2O are Iterative Reweighted Least Squares Method (IRLSM) and Limited-memory Broyden-Fletcher-Goldfarb-Shanno (L_BFGS). IRLSM uses a Gram Matrix approach underneath the hood, which is very efficient for tall and narrow datasets and when running lambda search with sparse solution. For wider and dense datasets (thousands of predictors and up), the L_BFGS solver scales better.

For performance reasons, we recommend not using any L1 penalty when using the L_BFGS solver, since model building can be slower. It is often better to run lambda search with IRLSM solver instead.

5.6.2 Stopping criteria

When using L1 penalty with lambda search, you can specify the `max_active_predictors` parameter to stop the search before it completes. Models built at the beginning of the lambda search have higher lambda values, consider fewer predictors, and take less time to calculate the model. Models built at the end of the lambda search have lower lambda values, incorporate more predictors, and take a longer time to calculate the model. You can also set the `nlambdas` parameter for a lambda search to specify the number of models attempted across the search.

Example in R

```
1 library(h2o)
2 h2o.init()
3 h2o_df = h2o.importFile("http://s3.amazonaws.com/h2o-public-test-
  data/smalldata/airlines/allyears2k_headers.zip")
4 model = h2o.glm(y = "IsDepDelayed", x = c("Year", "Origin"),
  training_frame = h2o_df, family = "binomial", lambda_search =
  TRUE, max_active_predictors = 10)
```

```
5 print(model)
6 v1 = model$model$coefficients
7 v2 = v1[v1 > 0]
8 print(v2)
```

Example in Python

```
1 import h2o
2 h2o.init()
3 h2o_df = h2o.import_file("http://s3.amazonaws.com/h2o-public-test
   -data/smalldata/airlines/allyears2k_headers.zip")
4 model = h2o.glm(y = "IsDepDelayed", x = ["Year", "Origin"],
   training_frame = h2o_df, family = "binomial", lambda_search =
   True, max_active_predictors = 10)
5 print(model)
6 #v1 = model$model$coefficients
7 #v2 = v1[v1 > 0]
8 #print(v2)
```

5.7 Advanced features

H2O's GLM has several advanced features to help build better models.

5.7.1 Standardizing data

The `standardize` parameter, which is enabled by default, standardizes numeric columns to have zero mean and unit variance. This parameter must be enabled (using `standardize=TRUE`) to produce standardized coefficient magnitudes in the model output.

We recommend enabling standardization when using regularization (i.e. `lambda` is chosen by H2O or set by the user to be greater than 0). Only advanced users should disable standardization.

5.7.2 N-fold 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.

You can also specify the rows that are assigned to each fold using the `fold_assignment` or `fold_column` parameters.

Example in R

```

1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 h2o_df$CAPSULE = as.factor(h2o_df$CAPSULE)
6 binomial.fit = h2o.glm(y = "CAPSULE", x = c("AGE", "RACE", "PSA",
      "GLEASON"), training_frame = h2o_df, family = "binomial",
      nfolds = 5)
7 print(binomial.fit)
8 print(paste("training_auc: ", binomial.fit@model$training_
      metrics@metrics$AUC))
9 print(paste("cross-validation_auc: ", binomial.fit@model$cross_
      validation_metrics@metrics$AUC))

```

5.7.3 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, specifying only a few values is typically 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 very 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, we recommend running with $alpha = 1 - \epsilon$ instead.

Example in R

```

1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 h2o_df$CAPSULE = as.factor(h2o_df$CAPSULE)
6 alpha_opts = list(list(0), list(.25), list(.5), list(.75), list
      (1))
7 hyper_parameters = list(alpha = alpha_opts)
8 grid <- h2o.grid("glm", hyper_params = hyper_parameters,
9      y = "CAPSULE", x = c("AGE", "RACE", "PSA", "
      GLEASON"), training_frame = h2o_df, family = "
      binomial")
10 grid_models <- lapply(grid@model_ids, function(model_id) { model
      = h2o.getModel(model_id) })

```

```

11 for (i in 1:length(grid_models)) {
12     print(sprintf("regularization: %-50s auc: %f", grid_models[[
        i]]@model$model_summary$regularization, h2o.auc(grid_models
        [[i]])))
13 }

```

5.7.4 Grid search over lambda

Grid search over lambda is a feature from H2O-2 that is not currently supported in H2O-3. Instead, use the built-in lambda search capability in GLM.

5.7.5 Offsets

`offset_column` is an optional column name or index referring to a column in the training frame. This column specifies a prior known component to be included in the linear predictor during training. 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.

5.7.6 Row weights

`weights_column` is an optional column name or index referring to a column in the training frame. This column specifies on a per-row basis the weight of that row. If no weight column is specified, a default value of 1 is used for each row. 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.

5.7.7 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

5.7.8 Proximal operators

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 GLM Model Output

The following sections explain the output produced by logistic regression (i.e. binomial classification).

Example in R

```

1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 h2o_df$CAPSULE = as.factor(h2o_df$CAPSULE)
6 rand_vec <- h2o.runif(h2o_df, seed = 1234)
7 train <- h2o_df[rand_vec <= 0.8,]
8 valid <- h2o_df[rand_vec > 0.8,]
9 binomial.fit = h2o.glm(y = "CAPSULE", x = c("AGE", "RACE", "PSA",
      "GLEASON"), training_frame = train, validation_frame = valid,
      family = "binomial")
10 print(binomial.fit)

```

```

1 Model Details:
2 =====
3
4 H2OBinomialModel: glm
5 Model ID: GLM_model_R_1439511782434_25
6 GLM Model:
7   family link regularization
8   number_of_predictors_total number_of_active_predictors
9   number_of_iterations training_frame
10 1 binomial logit Elastic Net (alpha = 0.5, lambda = 4.674E-4 )
      4
      5 subset_39
9
10 Coefficients:

```

```

11      names coefficients standardized_coefficients
12 1 Intercept      -6.467393                -0.414440
13 2      AGE       -0.021983                -0.143745
14 3      RACE      -0.295770                -0.093423
15 4      PSA       0.028551                 0.604644
16 5      GLEASON   1.156808                 1.298815
17
18 H2OBinomialMetrics: glm
19 ** Reported on training data. **
20
21 MSE:  0.1735008
22 R^2:  0.2842015
23 LogLoss:  0.5151585
24 AUC:  0.806806
25 Gini:  0.6136121
26 Null Deviance:  403.9953
27 Residual Deviance:  307.0345
28 AIC:  317.0345
29
30 Confusion Matrix for F1-optimal threshold:
31      0      1      Error      Rate
32 0      125   50 0.285714  =50/175
33 1       24   99 0.195122  =24/123
34 Totals 149 149 0.248322  =74/298
35
36 Maximum Metrics:
37      metric threshold      value idx
38 1      max f1  0.301518 0.727941 147
39 2      max f2  0.203412 0.809328 235
40 3      max f0point5 0.549771 0.712831 91
41 4      max accuracy 0.301518 0.751678 147
42 5      max precision 0.997990 1.000000 0
43 6      max absolute_MCC 0.301518 0.511199 147
44 7 max min_per_class_accuracy 0.415346 0.739837 134
45
46 H2OBinomialMetrics: glm
47 ** Reported on validation data. **
48
49 MSE:  0.1981162
50 R^2:  0.1460683
51 LogLoss:  0.5831277
52 AUC:  0.7339744
53 Gini:  0.4679487
54 Null Deviance:  108.4545
55 Residual Deviance:  95.63294
56 AIC:  105.6329

```



```

57
58 Confusion Matrix for F1-optimal threshold:
59      0  1  Error  Rate
60 0      35 17 0.326923 =17/52
61 1       8 22 0.266667 =8/30
62 Totals 43 39 0.304878 =25/82
63
64 Maximum Metrics:
65      metric threshold  value  idx
66 1      max f1  0.469237 0.637681  38
67 2      max f2  0.203366 0.788043  63
68 3      max f0point5 0.527267 0.616438  28
69 4      max accuracy 0.593421 0.719512  18
70 5      max precision 0.949357 1.000000   0
71 6      max absolute_MCC 0.469237 0.391977  38
72 7 max min_per_class_accuracy 0.482906 0.692308  36

```

6.1 Coefficients and normalized coefficients

Coefficients are the predictor weights (i.e. the actual model used for prediction). Coefficients should be used to make predictions for new data points:

```
1 binomial.fit@model$coefficients
```

```

1      Intercept      AGE      RACE      PSA      GLEASON
2 -6.46739299 -0.02198278 -0.29576986 0.02855057 1.15680761

```

If the `standardize` option is enabled, H2O returns another set of coefficients: the standardized 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 “normal” coefficients are obtained from the standardized 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.

Standardized coefficients are useful for comparing the relative contribution of different predictors to the model:

```
1 binomial.fit@model$coefficients_table
```

```

1 Coefficients:
2      names coefficients standardized_coefficients
3 1 Intercept      -6.467393                -0.414440
4 2      AGE      -0.021983                -0.143745
5 3      RACE      -0.295770                -0.093423

```

6	4	PSA	0.028551	0.604644
7	5	GLEASON	1.156808	1.298815

This view provides a sorted list of standardized coefficients in descending order for easy comparison:

```
1 binomial.fit@model$standardized_coefficient_magnitudes
```

```
1 Standardized Coefficient Magnitudes:
2      names coefficients sign
3 GLEASON GLEASON      1.298815 POS
4 PSA      PSA      0.604644 POS
5 AGE      AGE      0.143745 NEG
6 RACE      RACE      0.093423 NEG
```

6.2 Model statistics

Various model statistics are available:

MSE is the mean squared error: $MSE = \frac{1}{N} \sum_{i=1}^N (actual_i - prediction_i)^2$

R² is the R squared: $R^2 = 1 - \frac{MSE}{\sigma_y^2}$

LogLoss is the log loss. $LogLoss = \frac{1}{N} \sum_i \sum_j y_i \log(p_{i,j})$

AUC is available only for binomial models and is defined the area under ROC curve.

Gini TODO

Null deviance Deviance (defined by selected family) computed for the null model.

Residual deviance Deviance of the built model

AIC is based on log-likelihood, which is summed up similarly to deviance

Fetch these statistics using the following accessor functions:

```
1 h2o.num_iterations(binomial.fit)
2 h2o.null_dof(binomial.fit, train = TRUE, valid = TRUE)
3 h2o.residual_dof(binomial.fit, train = TRUE, valid = TRUE)
4
5 h2o.mse(binomial.fit, train = TRUE, valid = TRUE)
6 h2o.r2(binomial.fit, train = TRUE, valid = TRUE)
7 h2o.logloss(binomial.fit, train = TRUE, valid = TRUE)
8 h2o.auc(binomial.fit, train = TRUE, valid = TRUE)
9 h2o.giniCoef(binomial.fit, train = TRUE, valid = TRUE)
10 h2o.null_deviance(binomial.fit, train = TRUE, valid = TRUE)
11 h2o.residual_deviance(binomial.fit, train = TRUE, valid = TRUE)
12 h2o.aic(binomial.fit, train = TRUE, valid = TRUE)
```

6.3 Confusion matrix

Fetch the confusion matrix directly using the following accessor function:

```
1 h2o.confusionMatrix(binomial.fit, valid = FALSE)
2 h2o.confusionMatrix(binomial.fit, valid = TRUE)
```

6.4 Scoring history

The following output example represents a sample scoring history:

```
1 binomial.fit@model$scoring_history
```

```
1 Scoring History:
2           timestamp    duration iteration log_likelihood
3           objective
4 1 2015-08-13 19:05:17 0.000 sec           0           201.99764
5           0.67784
6 2 2015-08-13 19:05:17 0.002 sec           1           158.46117
7           0.53216
8 3 2015-08-13 19:05:17 0.003 sec           2           153.74404
9           0.51658
10 4 2015-08-13 19:05:17 0.004 sec           3           153.51935
11           0.51590
12 5 2015-08-13 19:05:17 0.005 sec           4           153.51723
13           0.51590
14 6 2015-08-13 19:05:17 0.006 sec           5           153.51723
15           0.51590
```

7 Making Predictions

Once you have built a model, you can use it to make predictions using two different approaches: the in-H2O batch scoring approach and the real-time NanoFast POJO approach.

7.1 Batch in-H2O predictions

Batch in-H2O predictions are made using a normal H2O cluster on a new H2OFrame. In addition to predictions, you can also get metrics like AUC if you include the response column in the new data. Refer to the following example for logistic regression (i.e. binomial classification).

Example in R

```

1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 h2o_df$CAPSULE = as.factor(h2o_df$CAPSULE)
6 rand_vec <- h2o.runif(h2o_df, seed = 1234)
7 train <- h2o_df[rand_vec <= 0.8,]
8 valid <- h2o_df[(rand_vec > 0.8) & (rand_vec <= 0.9),]
9 test <- h2o_df[rand_vec > 0.9,]
10 binomial.fit = h2o.glm(y = "CAPSULE", x = c("AGE", "RACE", "PSA",
      "GLEASON"), training_frame = train, validation_frame = valid,
      family = "binomial")
11
12 # Make and export predictions.
13 pred = h2o.predict(binomial.fit, test)
14 h2o.exportFile(pred, "/tmp/pred.csv", force = TRUE)
15 # Or you can export the predictions to hdfs:
16 #   h2o.exportFile(pred, "hdfs://namenode/path/to/file.csv")
17
18 # Calculate metrics.
19 perf = h2o.performance(binomial.fit, test)
20 print(perf)

```

Here is an example of making predictions on new data:

```

1 # Remove the response column to simulate new data points arriving
  without the answer being known.
2 newdata = test
3 newdata$CAPSULE <- NULL
4 newpred = h2o.predict(binomial.fit, newdata)
5 head(newpred)

```

	predict	p0	p1
1	1	0.1676892	0.8323108
2	0	0.4824181	0.5175819
3	1	0.2000061	0.7999939
4	0	0.9242169	0.0757831
5	0	0.5044669	0.4955331
6	0	0.7272743	0.2727257

The three columns in the prediction file are the predicted class, the probability that the prediction is class 0, and the probability that the prediction is class 1. The predicted class is chosen based on the maximum-F1 threshold.

You can change the threshold manually, for example to 0.3, and recalculate the predict column like this:

```

1 newpred$predict = newpred$p1 > 0.3
2 head(newpred)

```

```

1   predict      p0      p1
2 1         1 0.1676892 0.8323108
3 2         1 0.4824181 0.5175819
4 3         1 0.2000061 0.7999939
5 4         0 0.9242169 0.0757831
6 5         1 0.5044669 0.4955331
7 6         0 0.7272743 0.2727257

```

7.2 Low-latency predictions with the NanoFast scoring engine

For NanoFast scoring, H2O GLM models can be directly rendered as a Plain Old Java Object (POJO). These are very low latency and can easily be embedded in any Java environment (a customer-facing web application, a Storm bolt, or a Spark Streaming pipeline, for example).

The POJO does nothing but pure math, and has no dependencies on any other software packages (not even H2O itself), so it is easy to work with.

Directions for using the POJO in detail are beyond the scope of this document, but here is an example of how to get one and view it. You can also access the POJO from the Flow Web UI.

Example in R

```

1 library(h2o)
2 h2o.init()
3 path = system.file("extdata", "prostate.csv", package = "h2o")
4 h2o_df = h2o.importFile(path)
5 h2o_df$CAPSULE = as.factor(h2o_df$CAPSULE)
6 binomial.fit = h2o.glm(y = "CAPSULE", x = c("AGE", "RACE", "PSA",
7       "GLEASON"), training_frame = h2o_df, family = "binomial")
8 h2o.download_pojo(binomial.fit)

```

8 Best Practices

Here are a few rules of thumb to follow:

- The IRLSM solver works best on tall and skinny datasets
- If you have a wide dataset, use an L1 penalty to eliminate columns from the model
- If you have a wide dataset, try the L_BFGS solver

- When trying lambda search, specify `max_predictors` if it is taking too long. 90% of the time is spent on the larger models with the small lambdas, so specifying `max_predictors` helps a lot
- Retain a small L2 penalty (i.e. ridge regression) for numerical stability (i.e. don't use `alpha` 1.0, use 0.95 instead)
- Use symmetric nodes in your H2O cluster
- For the IRLSM solver, bigger nodes can help the ADMM / Cholesky decomposition run faster
- If you need to impute data, do so before running GLM

8.1 Verifying Model Results

To determine the accuracy of your model:

- Look for suspiciously different cross-validation results between folds

Example in R

```

1 library(h2o)
2 h2o.init()
3 h2o_df = h2o.importFile("http://s3.amazonaws.com/h2o-public-
  test-data/smalldata/airlines/allyears2k_headers.zip")
4 model = h2o.glm(y = "IsDepDelayed", x = c("Year", "Origin"),
  training_frame = h2o_df, family = "binomial", nfolds = 5)
5 print(paste("full_model_training_auc:", model@model$training_
  metrics@metrics$AUC))
6 print(paste("full_model_cv_auc:", model@model$cross_validation_
  metrics@metrics$AUC))
7 for (i in 1:5) {
8   cv_model_name = model@model$cross_validation_models[[i]]$
    name
9   cv_model = h2o.getModel(cv_model_name)
10  print(paste("cv_fold_", i, "_training_auc:", cv_
    model@model$training_metrics@metrics$AUC, "_validation_
    auc:", cv_model@model$validation_metrics@metrics$AUC))
11 }

```

- Look for explained deviance ($1 - \frac{NullDev - ResDev}{NullDev}$)
 - Too close to 0: model doesn't predict well
 - Too close to 1: model predicts too well (one of your input columns is probably a cheating column)
- For logistic regression (i.e. binomial classification) models, look for AUC

- Too close to 0.5: model doesn't predict well
- Too close to 1: model predicts too well
- Look at the `number_of_iterations` or scoring history to see if GLM stops early for a particular `lambda` that interests you (performing all the iterations probably means the solution is not good). This is controlled by the `max_iterations` parameter.
- Too many NAs in your training data is bad (GLM discards rows with NA values) You should always check degrees of freedom of the output model. Degrees of freedom is number of observations used to train the model minus the size of the model. If this number is way smaller than expected, it is likely that too many rows have been excluded due to having missing values.
 - If you have few columns with many NAs, you might accidentally be losing all your rows and it's better to exclude them.
 - If you have many columns with small fraction of uniformly distributed missing values, every row is likely going to have at least one missing value. In this case, NAs should be imputed (filled in, e.g. with mean) before modelling.

9 Implementation Details

The following sections discuss some of the implementation choices in H2O's GLM.

9.1 Categorical variables

When applying linear models to datasets with categorical variables, the usual approach is to expand the categorical 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.

9.1.1 Largest categorical speed optimization

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 Cholesky 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.

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

9.2 Speed and memory performance characteristics

This section discusses the CPU and memory cost of running GLM for each available solver.

9.2.1 IRLSM solver

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:

	CPU	Memory
Gram matrix ($X^T X$) (distributed)	$O(\frac{MN^2}{pn})$	$O(\text{training data}) + O(\text{gram matrix})$ $O(MN) + O(N^2pn)$
ADMM + Cholesky decomposition (single node)	$O(\frac{N^3}{p})$	$O(N^2)$

- M Number of rows in the training data
 N Number of predictors in the training data
 p Number of CPUs per node
 n Number of nodes in the cluster

If $M \gg N$, the algorithm scales linearly both in the number of nodes and the number of CPUs per node. However, the 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.

9.2.2 L-BFGS solver

In each iteration, L-BFGS computes a gradient at the current vector of coefficients and then computes an updated vector of coefficients in an approximated Newton-method step. The cost of the coefficient update is $k*N$, where N is number of predictors and k is a constant, the cost of gradient computation is $\frac{M*N}{pn}$ where M is number of observations in the dataset and pn is the number of cpu cores in the cluster. Since k is a (small) constant, the runtime of L-BFGS is dominated by the gradient computation, which is fully parallellized and L-BFGS thus scales almost linearly.

9.3 Data corner cases

- What if: the training data has an NA? All rows conatining (any) missing value are omitted form the training set.
- What if: the test data has an NA? The prediction for that observation is NA.
- What if: a predictor column is categorical, you are making predictions on test data, and the predictor is a level that wasn't seen during training? The value is zero for all predictors associated with the particular categorical vairable.
- What if: the response column is categorical, you are making predictions on test data, and the response is a level that wasn't seen during training? Only binomial model is supported, any extra levels in test-response will trigger an error.

10 H2O Community Resources

For more information about H2O, visit the following open-source sites:

H2O Full Documentation: <http://docs.h2o.ai>

H2O-3 Github Repository: <https://github.com/h2oai/h2o-3>

Open-source discussion forum: h2ostream@googlegroups.com
<https://groups.google.com/d/forum/h2ostream>

Issue tracking: <http://jira@h2o.ai>

To contact us securely and privately, email us at support@h2o.ai.

11 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-05.

- `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.
- `n_lambdas`: 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 -1.0.
- `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.

References

- [1] Jerome Friedman, Trevor Hastie, and Rob Tibshirani. **Regularization Paths for Generalized Linear Models via Coordinate Descent**. April 29, 2009
- [2] Robert Tibshirani, Jacob Bien, Jerome Friedman, Trevor Hastie, Noah Simon, Jonathan Taylor, and Ryan J. Tibshirani. **Strong Rules for Discarding Predictors in Lasso-type Problems**. J. R. Statist. Soc. B, vol. 74, 2012.
- [3] Hui Zou and Trevor Hastie **Regularization and variable selection via the elastic net**. J. R. Statist. Soc. B (2005) 67, Part 2, pp. 301-320
- [4] Robert Tibshirani. **Regression Shrinkage and Selection via the Lasso** Journal of the Royal Statistical Society. Series B (Methodological), Volume 58, Issue 1 (1996), 267-288
- [5] S. Boyd, N. Parikh, E. Chu, B. Peleato, and J. Eckstein. **Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers**. Foundations and Trends in Machine Learning, 3(1):1122, 2011. (Original draft posted November 2010.)
- [6] N. Parikh and S. Boyd. **Proximal Algorithms**. Foundations and Trends in Optimization, 1(3):123-231, 2014.
- [7] <http://github.com/h2oai/h2o.git>
- [8] <http://docs.h2o.ai>
- [9] <https://groups.google.com/forum/#!forum/h2ostream>
- [10] <http://h2o.ai>
- [11] <https://0xdata.atlassian.net/secure/Dashboard.jspa>