Cluster Analysis with the BigML Dashboard

The BigML Team

Version 1.2



MACHINE LEARNING MADE BEAUTIFULLY SIMPLE

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About this Document

This document provides a comprehensive description of how to solve cluster analysis using the BigML Dashboard. BigML Clusters are covered in detail. Learn how to use the BigML Dashboard to configure, visualize, and interpret these unsupervised predictive models and use them to find centroids for single instances and whole datasets as well.

This document assumes that you are familiar with:

- Sources with the BigML Dashboard. The BigML Team. June 2016. [6]
- Datasets with the BigML Dashboard. The BigML Team. June 2016. [5]

To learn how to use the BigML Dashboard to build supervised predictive models read:

- Classification and Regression with the BigML Dashboard. The BigML Team. June 2016. [4]
- Time Series with the BigML Dashboard. The BigML Team. July 2017. [7]

To learn how to use the BigML Dashboard to build other unsupervised models read:

- Anomaly Detection with the BigML Dashboard. The BigML Team. June 2016. [2]
- Association Discovery with the BigML Dashboard. The BigML Team. June 2016. [3]
- Topic Modeling with the BigML Dashboard. The BigML Team. November 2016. [8]

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CHAPTER

Introduction

There are problems that require separating datasets into subsets of instances bearing some similarities. Cluster analysis is a Machine Learning task that partitions a dataset and groups together those instances that are similar. It separates a set of instances into a number of groups so that instances in the same group, called cluster, are more similar to each other than to those in other groups. Cluster analysis does not require using previously labeled data. For this reason, it falls under the category of unsupervised learning.

BigML clusters use proprietary learning algorithms to group together the instances according to a distance measure, computed using the values of the fields as input. Each cluster group is represented by its center (or centroid). All BigML field types are valid inputs for clustering, i.e. categorical, numeric, text and items fields, although there are a few caveats. First, numeric fields are automatically scaled to ensure that their different magnitudes do not bias the distance calculation. Second, clustering does not tolerate missing values for numeric fields, so BigML provides several strategies for dealing with them (see Section 4.4), otherwise those instances are excluded to compute the clusters.

BigML clusters can be built using two different unsupervised learning algorithms:

- K-means: the user needs to specify the number of clusters in advance. Learn more about k-means in Section 2.1.
- **G-means**: the algorithm automatically learns the number of different clusters by iteratively taking existing cluster groups and testing whether the cluster's neighborhood appears Gaussian in its distribution. Learn more about g-means in Section 2.2.

This chapter provides a comprehensive description of BigML clusters including how they can be created (Chapter 3) and configured (Chapter 4). Powerful visualizations are provided of the results of clustering data instances, which give insight into their internal structure (see Chapter 5). Besides their visual representations, clusters also provide a textual summary view of the most essential information about them (see Chapter 6). Clusters are actionable, since they allow you to identify the cluster that is closest to any given new data point (Chapter 7). You can even download and calculate the nearest cluster locally (see Section 8.1). It is also worth noting that you can create, update, list, and delete clusters using the BigML API (see Section 8.3).

In BigML, the fourth tab of the main menu of your <code>Dashboard</code> allows you to list all your available clusters. In the cluster list view (Figure 1.2), you can see, for each cluster, the <code>dataset</code> it was created from, as well as the cluster's <code>Name</code>, <code>Algorithm</code> (either k-means or g-means), the number of cluster groups <code>K</code>, <code>Age</code> (time elapsed since it was created), <code>Size</code>, and number of <code>centroids</code> or <code>batch centroids</code> that have been created using that cluster. The <code>SEARCH</code> menu option in the top right corner of the cluster list view allows you to search your clusters by name.

1



Figure 1.1: Clusters list view

When you first create an account at BigML, or every time you start a new project, your list view of clusters will be empty. (See Figure 1.2.)



Figure 1.2: Empty Dashboard cluster view

Finally, in Figure 1.3 you can see the icon used to represent a cluster in BigML.



Figure 1.3: Cluster icon

Understanding Clusters

This section describes internal details about BigML clusters. Besides being useful to better understand how BigML implements them, it will also provide the foundations for you to decide why and when to use the two available clustering algorithms. You can safely skip this section on first read.

2.1 K-Means

K-means is one of two algorithms that BigML provides for cluster analysis. K-means clustering aims to partition the data instances contained in your dataset in K clusters, such that each data instance belongs to the cluster with the nearest center.

BigML proprietary implementation of K-means is optimized for scalability, thus mitigating one of the major limitations of standard K-means. BigML adopted the mini-batch¹ approach, which is known to reduce computation cost by orders of magnitude compared to the classic K-means algorithm.

One key factor when using K-means clustering is how the algorithm is initialized, which can greatly affect the quality of the identified clusters. In standard K-means, initial clusters are chosen at random. This means that the quality of the clusters identified by the algorithm usually varies a lot from run to run, so it is fair to say that standard K-means provides no guarantee of accuracy². Therefore, alternative approaches for the selection of the initial clusters have been described in literature, such as K-means++, which is a little too slow for BigML purposes. Instead, BigML preferred approach is K-means ||³, which is similar to K-means++ but much faster.

Another dimension where BigML clusters improve on standard K-means is the way they handle categorical data. Instead of "binarizing" each category, meaning a field with 40 categories becomes 40 binary fields, BigML chose a technique called k-prototypes⁴ which modifies the distance function to be more category-friendly so each cluster chooses the most common category from its neigborhood. So, BigML Clusters use mode instead of mean for categorical fields.

2.2 G-Means

Sometimes, it is hard to know in advance how many clusters can be identified in a given dataset (the K in K-means). To solve this issue, an alternative algorithm has been proposed, G-means⁵, which uses a special technique for running K-means multiple times while adding centroids in a hierarchal fashion. G-means has the advantage of being relatively resilient to covariance in clusters and has no need to

¹http://www.eecs.tufts.edu/~dsculley/papers/fastkmeans.pdf

²http://ilpubs.stanford.edu:8090/778/1/2006-13.pdf

 $^{^{3} \}texttt{http://theory.stanford.edu/\%7Esergei/papers/vldb12-kmpar.pdf}$

 $[\]frac{4}{1}$ http://www.iipl.fudan.edu.cn/%7Ezhangjp/literatures/cluster%20analysis/apkdd.pdf

⁵http://papers.nips.cc/paper/2526-learning-the-k-in-k-means.pdf

compute a global covariance (as is the case with using the Mahalanobis⁶ distance, a popular variant on classic K-means to deal with covariance).

BigML implementation differs from the original paper. First, we reuse our sample-based K-means rather than running full K-means, with the already described performance and scalability advantage. Additionally, BigML clusters choose new candidate clusters with kmeans|| rather than the PCA calculation from the paper. While this gives us better scalability, it means BigML version of G-means is no longer deterministic as in the paper. Given the same data, we may find a different number of clusters from one run to the next (if no seed is given).

Finally, BigML G-means have different stopping criteria than the original paper. We currently enforce a maximum limit of 128 clusters. Also, if BigML algorithm does not make sufficient progress in finding Gaussian clusters after multiple iterations of G-means, it stops early. Both techniques ensure that BigML algorithm returns fewer clusters.

G-means is almost parameter-free, except for one, the critical_value parameter. G-means iteratively takes existing clusters and tests whether the cluster's neighborhood appears Gaussian. If it does not, the cluster is split into two. The critical_value sets how strict the test is when deciding whether data looks Gaussian. The current default is 5, but ranges between 1 and 20 can be reasonable depending on the dataset. A critical value of 1 means data must look very Gaussian to pass the test and can lead to more clusters being detected. Higher critical_values will tend to find fewer clusters.

2.3 On the Repeatability of Clusters

As mentioned, standard K-means provides results that vary strongly from run to run due to the random selection of initial clusters. However, BigML clusters strive to ensure that obtained results are repeatable, to some extent. In particular, when applying K-means||, BigML will ensure that the same initial cluster selection is done for each given dataset.

As an end effect, if you choose the K-means algorithm, BigML Clusters are repeatable when you use the same dataset to create them. Alternatively, if you create different datasets from the same datasource, no guarantee can be provided as to the repeatability of the results.

The same considerations apply to BigML G-means repeatability.

2.4 Clusters with Images

Image obviously is one of the most important categories among all data, and its presence is ever increasing. It is estimated that more than 85% of all Internet traffic today are visual data. Research also indicates that 90% of the information transmitted to human brain is visual. Therefore it's very important to support and develop machine learning with images.

BigML extracts image features at the source level. Image features are sets of numeric fields for each image. They can capture parts or patterns of an image, such as edges, colors and textures. BigML also supports image features extracted by pre-trained CNNs which capture more sophisticated features. Depending on different machine learning use cases and goals, all these image features can be effective in cluster analysis, as well as other unsupervised and supervised models.

For information about the image features, please refer to section Image Analysis of the Sources with the BigML Dashboard⁷[6].

⁶https://en.wikipedia.org/wiki/Mahalanobis_distance

⁷https://static.bigml.com/pdf/BigML_Sources.pdf

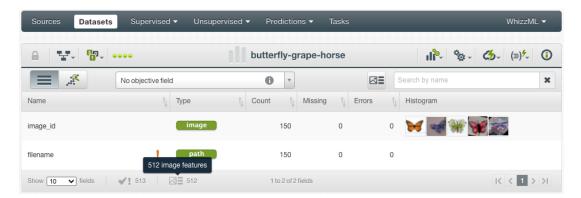


Figure 2.1: A dataset with images and image features

As shown in Figure 2.1, the example dataset has an image field <code>image_id</code>. It also has image features extracted from the images referenced by <code>image_id</code>. Image feature fields are hidden by default to reduce clutter. To show them, click on the icon "Click to show image features", which is next to the "Search by name" box. In Figure 2.2, the example dataset has 512 image feature fields, extracted by a pre-trained CNN, <code>ResNet-18</code>.

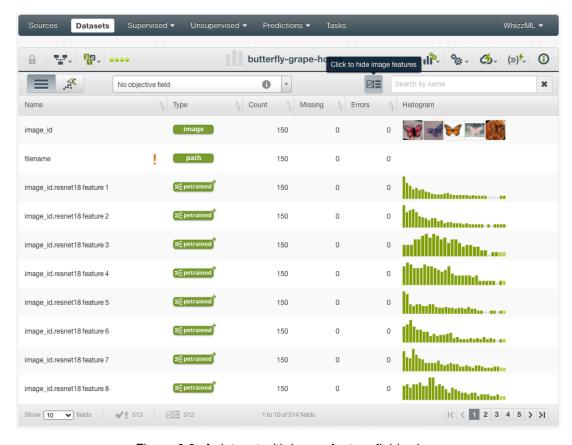


Figure 2.2: A dataset with image feature fields shown

From image datasets like this, clusters can be created and configured using the steps described in the following chapters.

Creating Clusters with 1-Click

To create a cluster in BigML you have two options: you can use the BigML unique **1-click** feature which provides a convenient way to create a cluster from a dataset, or you can **configure** a number of options that give you fine control on how the cluster is created. This section will guide you through the process of creating a cluster with just 1-click.

By far, the easiest and quickest way to create a cluster is using the 1-CLICK CLUSTER option that is available in the **1-click action menu**. (See Figure 3.1.)



Figure 3.1: 1-click cluster

Alternatively, you can select the 1-CLICK CLUSTER option in the **1-click action menu** from the dataset list view. (See Figure 3.2.)

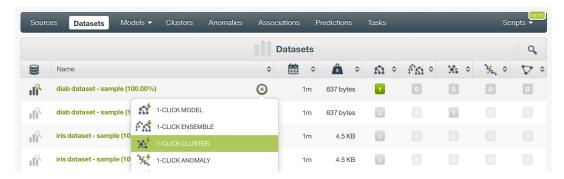


Figure 3.2: Pop up menu option to create a 1-click cluster from list view

Either option builds a new cluster using default values for all available configuration options (see Chapter 4). This can give you a quick starting point to understand how your clustering behaves and how to improve it.

Creating a cluster may take a variable time, depending on how big your dataset is, your subscription plan, etc. Once your clusuter is ready, it will be automatically displayed on your BigML Dashboard and

you will be able to explore it through BigML sophisticated visualizations (see Chapter 5,) and using it for predictions (see Chapter 7.)

Cluster Configuration Options

While 1-click creation (see Chapter 3) provides a convenient and easy way to create a cluster from a dataset, there are cases when you want more control. This section will focus on the options that BigML offers to configure its internal algorithms for clustering.

You can set a number of parameters that affect the way BigML creates models from a dataset. Such parameters can be grouped in two categories:

- Parameters that are permanently associated to the dataset, such as its objective field and preferred fields. Once you provide a value for a dataset's permanent parameters, they will be used as a default value for the creation of models from that dataset.
- Parameters that only affect the model that is currently being created and that you are expected to set each time. Those include the objective field, included/excluded fields, and a number of configuration options that are described below.

Set a dataset's permanent parameters by clicking on the edit button that is displayed when you hover on the dataset's fields. This opens a modal dialog where you can set some of the field properties (See Figure 4.1).

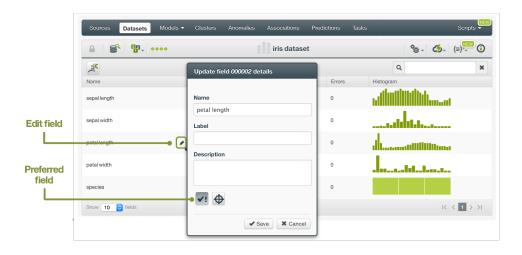


Figure 4.1: Configure permanent parameter modal

Click on the preferred field button to make that field non-preferred.

To access the **configuration panel**, select the CONFIGURE CLUSTERZ menu option located in the **configuration menu** of your dataset's detail view. (See Figure 4.2.)



Figure 4.2: Configure cluster

When the **configuration panel** is displayed, you can:

- Select or deselect individual fields for them to be included in or excluded from the cluster computation.
- · Set a number of configuration options.

Note: when the configuration panel is displayed, the edit is not visible, so you cannot set the dataset's permanent properties.

You can find a detailed explanation of the configuration options in the following sections.

4.1 Clustering Algorithms

BigML provides two distinct algorithms for clustering. Choose between K-means¹ and G-means² [1] to create your cluster. (See Figure 4.3.)

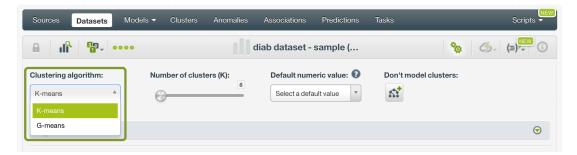


Figure 4.3: Cluster options: clustering algorithm

4.1.1 K-Means Algorithm

Using the κ -means algorithm requires that you already know the number of cluster groups (the κ in K-means) that are present in your dataset. If you do not know it, an inappropriate choice of κ may yield poor results.

The maximum number of clusters that you can specify is 300.

4.1.2 G-Means Algorithm

If you do not know which is the optimal number of cluster groups present in your dataset, you can have BigML discover it by using G-means. G-means solves the problem of trying to find the number of clusters by iteratively taking existing clusters and testing whether the cluster's neighborhood appears Gaussian in its distribution (based on Anderson-Darling tests³). See this blogpost⁴ for more information.

G-means will yield a maximum of 128 clusters.

4.2 Number of Clusters

When you select the K-means algorithm, you are required to configure the **number of clusters** that you know are to be found. (See Figure 4.4.)



Figure 4.4: Number of clusters

https://en.wikipedia.org/wiki/K-means_clustering

²http://papers.nips.cc/paper/2526-learning-the-k-in-k-means.pdf

³https://en.wikipedia.org/wiki/Anderson\T1\textendashDarling_test

 $^{^4}$ http://blog.bigml.com/2015/02/24/divining-the-k-in-k-means-clustering/

Note: choosing an inappropiate K can yield poor results. If you do not have any initial idea of how many clusters your data may contain, it is better to use G-means.

4.3 Critical Value

When you select the G-means algorithm, you can choose a critical value. (See Figure 4.5.)



Figure 4.5: Critical value options

The critical value determines how "strict" the G-means algorithm is when identifying clusters. When you select G-means, BigML iteratively tests new clusters looking for Gaussian distributions in the clusters' neighborhoods. If a new cluster does not pass the test, it is split into two new clusters. The critical value sets how strict this statistical test should be when deciding if the underlying data looks Gaussian. A critical value of 1 means the data must look very Gaussian to pass the test, so it can lead to more clusters being detected. Alternatively, higher critical values loosens the Gaussian constraint and leads to fewer clusters.

By default, BigML uses a value of 5, which seems to work well in most cases. A range between 1 and 10 is acceptable.

4.4 Default Numeric Value

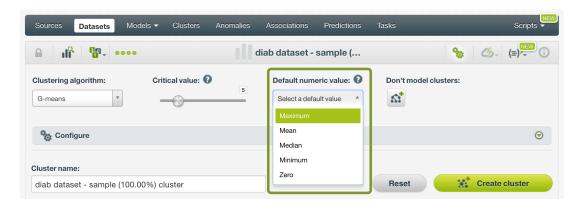


Figure 4.6: Cluster options: default numeric value

When training a cluster, BigML may encounter missing values, which can be either considered or ignored. Indeed, clusters compute the Euclidean distance⁵. Since the distance to a missing value is undefined, instances containing missing values will be ignored.

BigML. though, lets you use a default value in place of any missing value, by setting a default numeric value. You can choose to replace the missing numeric values with the field's maximum, mean, median, minimum or zero. There is one catch. If all the instances contain at least one missing value, this would invalidate the entire training set. In this situation, BigML automatically replaces the missing numeric values by the median.

 $^{^{5}}$ https://en.wikipedia.org/wiki/Euclidean_distance

Missing values for categorical fields are always considered valid categorical values, for example [red, green, blue, <missing>]. This means a cluster centroid may contain a missing value. (See Figure 4.7.)

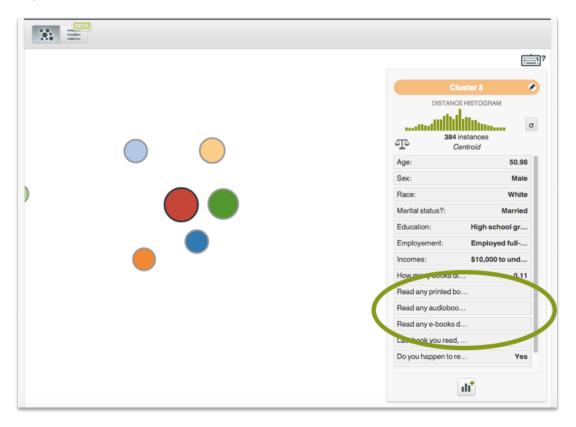


Figure 4.7: Example of a centroid with missing values for some categorical fields

4.5 Scale Fields & Auto-Scaled Fields

Datasets often contain fields with very different magnitudes. For example, two fields such as age and salary. Since clusters compute the Euclidean distance⁶ between numeric values, salary will dominate the clustering.

BigML provides two options to re-scale your fields (Figure 4.8):

- Scale fields: set a specific scale for your fields using an integer multiplier. This will increase their influence as many times as the number you set to calculate the clusters. If the auto-scaled option is enabled, it will be applied first so you can control how much weight you assign to a particular field relative to others. For example, if you want the age to be twice as influential as salary you just need to set auto-scaled to true and assign a multiplier of 2 to the age field.
- **Auto-scaling**: when the auto-scaled option is enabled, all the numeric fields will be scaled so that their standard deviations are 1. This ensures each field will have equal influence.

⁶https://en.wikipedia.org/wiki/Euclidean_distance

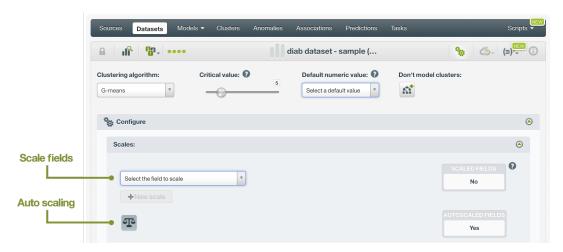


Figure 4.8: Cluster options: field scaling

4.6 Weights

This option allows you to assign individual weights to each instance by choosing a special weight field. This is useful when you have an unbalanced dataset, where data instances of given kind, e.g., those indicating a fraudulent transaction, are scarce in comparison to other ones. In such case, you may want to assign more **weight** to the scarce instances so they are equivalent to the abundant ones.

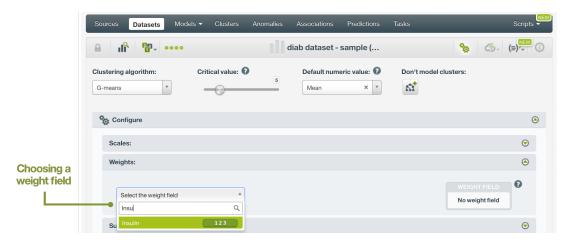


Figure 4.9: Cluster options: weight field

The selected field must be numeric, and it must not contain any missing values. The field selected for weighting purposes will not be taken into account as an input to calculate cluster distances. You can select an existing field in your dataset, or you can create a new one to assign customized weights.

For example, below you can find a transactional dataset example for which we included a field called "Weight". This field indicates that fraudulent instances weigh 10 more times than non fraudulent ones. BigML Flatline editor is a powerful tool for adding new fields to your dataset, such as a weight field. Another field that could be used in this example may be the transaction "Amount" so that transactions with higher amounts will have higher weights in the cluster.

Trans. ID	Products	Online	Amount \$	Fraud	Weight
xxxxxx098	XYZGH	yes	3,218	FALSE	1
xxxxxx345	VBHGF	no	1,200	FALSE	1
xxxxxx123	UYFHJ	yes	5,000	FALSE	1
xxxxxx567	HSNKI	no	390	FALSE	1
xxxxxx789	SHSYA	yes	500	TRUE	10
xxxxxx093	DFSTU	yes	423	FALSE	1
xxxxxx012	TYISJ	yes	60,000	FALSE	1
xxxxxx342	SJSOP	no	789	FALSE	1
xxxxxx908	IOPKJ	no	9,450	FALSE	1
xxxxxx334	HIOPN	yes	50,678	TRUE	10

Table 4.1: Weight Field example for transactional dataset

4.7 Sampling Options

Sometimes you do not need all the instances contained in your testing dataset to build your cluster. If you have a very large dataset, sampling may be a good way of getting faster results. (See Figure 4.10.)

The same sampling options described in the **Datasets with the BigML Dashboard document** [5] to sample datasets are also available when building clusters. They are divided in two groups: sampling and advanced sampling options.

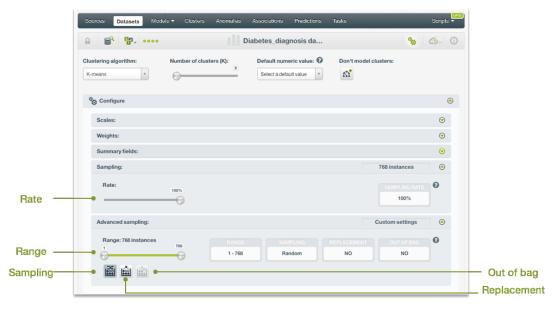


Figure 4.10: Sampling options for clusters

4.7.1 Rate

The sampling **rate** is the frequency of instances being extracted from the dataset and included in your sample. A sampling rate of 100% means that all instances are included; a rate of 10% means that only every tenth instance is included. This option may take any value between 0% and 100%. You can easily configure the **rate** by moving the slider in the **configuration panel for sampling**, or by typing the percentage in the tiny input box, both highlighted in Figure 4.10.

By default, BigML uses a 100% rate.

4.7.2 Range

The sampling **range** is the linear subset of the dataset instances that you want to include in the sample, e.g., from instance 5 to instance 1,000. The **rate** will be applied over the range configured.

By default, all instances are included, i.e., the range is (1, num. rows in dataset).

4.7.3 Sampling

The **sampling** option represents the type of the sampling process, which can be either random or deterministic.

When using deterministic sampling the random-number generator will always use the same seed, producing repeatable results.

By default, BigML uses random sampling.

4.7.4 Replacement

The **replacement** option controls whether a single instance can be selected multiple times or not. Sampling without replacement ensures that each instance cannot be selected more than once.

By default, BigML generates samples without replacement.

4.7.5 Out of Bag

The **out of bag** option allows you to include in your sample only those instances that were not selected in the first place, thus effectively inverting the sampling outcome. It is only selectable when a sample is deterministic and the sample rate is less than 100%. The total percentage of instances included in your sample will be one minus the **rate** (when replacement is not allowed). This can be useful for splitting a dataset into training and testing subsets.

By default, BigML will not use out of bag instances.

4.8 Creating Clusters with Configured Options

After finishing the configuration of your options, you can change the default cluster name in the editable text box. Then you can click on the Create cluster button to create the new cluster, or reset the configuration by clicking on the Reset button.



Figure 4.11: Create cluster after configuration

4.9 API Request Preview

The API Request Preview button is in the middle on the bottom of the configuration panel, next to the Reset button (See (Figure 4.11)). This is to show how to create the cluster programmatically: the endpoint of the REST API call and the JSON that specifies the arguments configured in the panel. Please see (Figure 4.12) below:

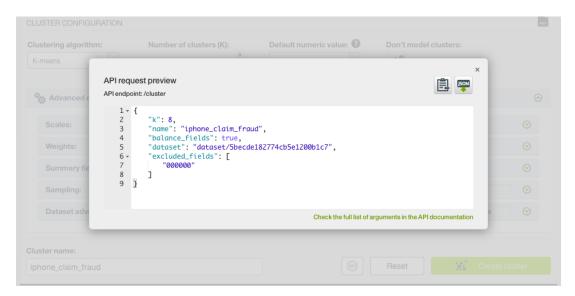


Figure 4.12: Cluster API request preview

There are options on the upper right to either export the JSON or copy it to clipboard. On the bottom there is a link to the API documentation for clusters, in case you need to check any of the possible values or want to extend your knowledge in the use of the API to automate your workflows.

Please note: when a default value for an argument is used in the chosen configuration, the argument won't appear in the generated JSON. Because during API calls, default values are used when arguments are missing, there is no need to send them in the creation request.

Visualizing Clusters

Being able to effectively visualize a model is of great help to understand how cluster groups relate one another. To this aim, BigML provides powerful interactive visualizations for clusters.

5.1 Cluster Visualization

BigML cluster visualization is available for all clusters. (See Figure 5.1.)

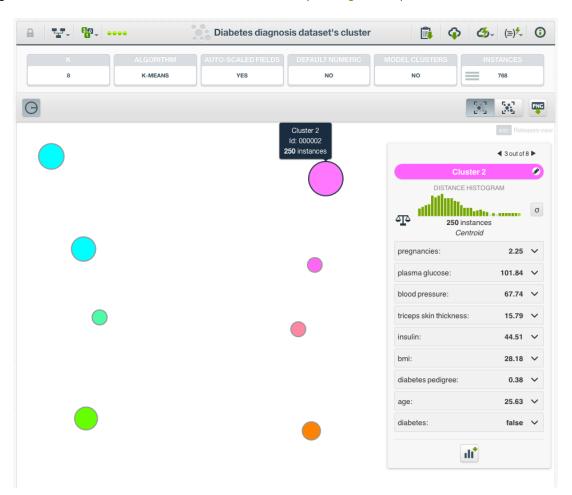


Figure 5.1: Clusters visualization

It conveys a wealth of information through a natural representation of cluster groups:

- Each cluster is associated to a circle, a standard representation for clusters.
- · Different cluster groups have different colors associated.
- The distances between clusters in the visualization is related to the actual distances. However, it is not strictly to scale, as to ensure that all clusters fit the screen. (See Figure 5.1.)
- When you mouse over a cluster, additional information will be displayed in a tooltip and in a **data** panel on the right side.

The tooltip includes the cluster name, ID, and the number of instances that it comprises.

The **data** panel shows the **distance histogram** (see Subsection 5.1.1) for the data points comprising that cluster as well as the **centroid** information Subsection 5.1.2). You can freeze the panel by pressing SHIFT; press ESCAPE to release the view.

If you click on the "Summary View" tab on the top right, the summary information of all the clusters will be listed in the panel on the right side. (See Figure 5.2.)

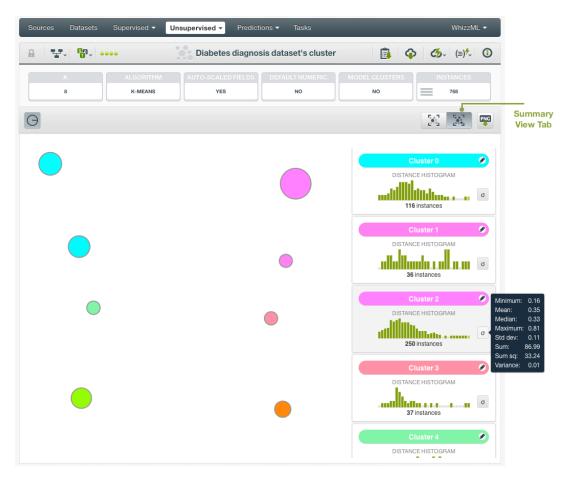


Figure 5.2: Summary view for clusters

The summary information includes the cluster name, its distance histogram and its number of instances. There may be more clusters than what are shown in the right panel, but if you mouse over a cluster in the diagram on the left, the panel will slide to show the corresponding cluster summary.

You can mouse over the cluster name bar to show its resource ID, or click on the pencil icon to edit the cluster name. In addition, you can mouse over a histogram to inspect its bins (ranges and instances), and mouse over the stats icon (sigma) to see the statistical summary of the instances in the cluster.

5.1.1 Distance Histogram

The distance histogram represents the distribution of distances from the cluster's center to each of the points that fall into the cluster's neighborhood.

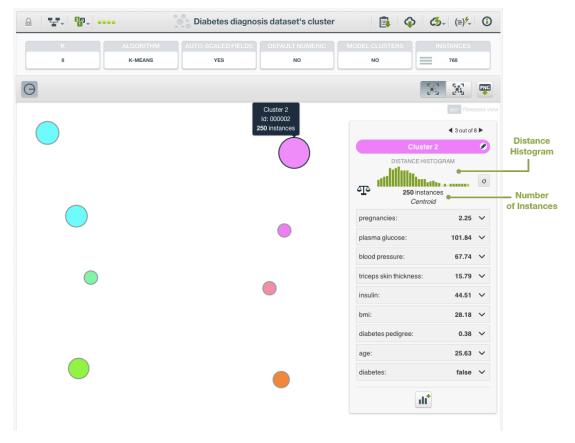


Figure 5.3: Distance histogram for clusters

5.1.2 Centroid

The cluster centroid is the center of the cluster. It is computed by using the mean for each numeric field and the mode for categorical ones.

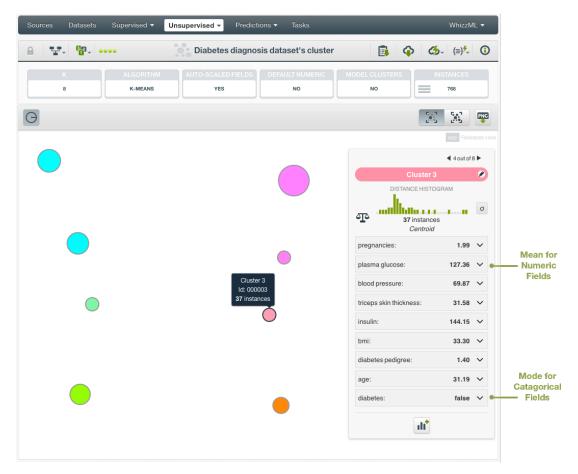


Figure 5.4: Centroid data inspector

For text and items fields, you will get a tag cloud where you can see the terms or items that minimize the average cosine distance between the centroid and the points in its neighborhood.



Figure 5.5: Centroid tag cloud for text and items fields

5.1.3 Cluster Visualization with Images

When clusters have images, their visualization is the same as described in the previous sections of this chapter. Additionally, there are image previews in the data panel.

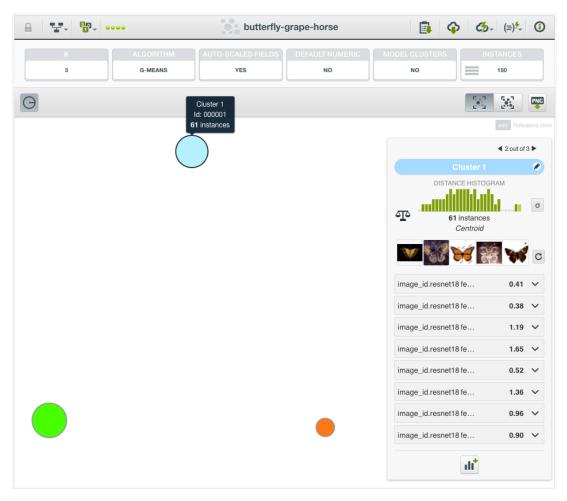


Figure 5.6: Cluster view with images

As shown in Figure 5.6, in the cluster view, when users mouse-over a cluster, its information will be displayed in a tooltip, as well as in the data panel on the right side. The data panel not only includes the distance histogram and the centroid information, it also presents a list of thumbnail images. The thumbnail images serve as previews of the images and can be changed by using the reloading icon next to them. Clicking on a thumbnail will bring up the close-up view of the image.

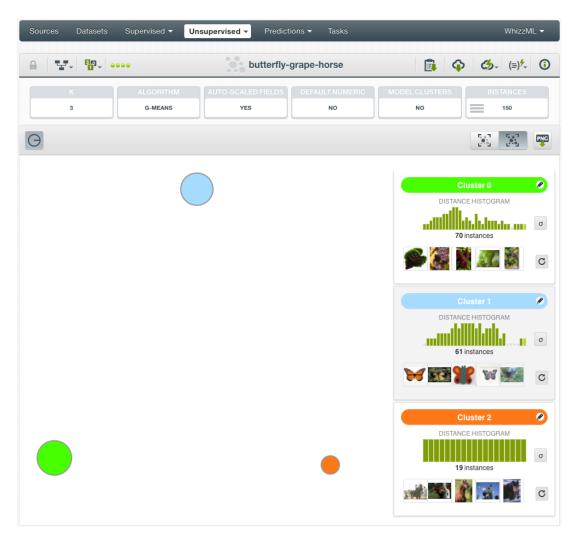


Figure 5.7: Cluster summary view with images

In the summary view, as shown in Figure 5.7, the data panel includes the cluster name, its distance histogram, its number of instances, as well as a list of thumbnail images as previews.

5.2 Creating a Dataset From a Cluster

Create a dataset from a cluster if you want to have all of the instances that belong to that cluster in a dataset for further analysis.

To create a dataset from a cluster, select the cluster by clicking it, then press SHIFT, and click the dataset icon at the bottom of your cluster's **data panel**.

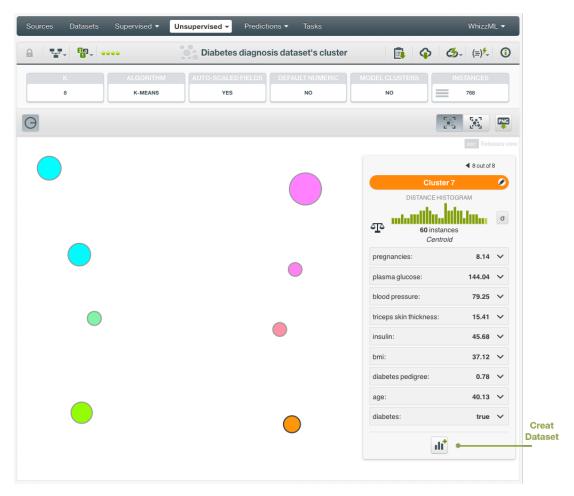


Figure 5.8: Create a dataset from a cluster

Cluster Summary Report

From a cluster's detail view, access the cluster summary report by clicking on the icon highlighted in Figure 6.1.



Figure 6.1: Button to display a cluster's summary report

The cluster summary report displays a summary about the cluster.

6.1 Cluster Summary

The cluster summary gives you a summarized view of your cluster, including the following metrics: data distribution, cluster metrics, centroids, and intercentroid distance. (See Figure 6.2.)

- **Data distribution**: data distribution within the clusters: for each cluster, the percentage of data instances that belong to that cluster is given. The "global" cluster always includes all of the data instances, i.e. it accounts for 100% of them.
- **Cluster metrics**: a summary of the distances between the data instances expressed in terms of various aggreagate measures:
 - total_ss: the total sum of squares of the distances between each data instance and the global centroid;
 - within_ss: the total sum of squares of the distances between each data instance and the centroid it belongs to;
 - between_ss: the total sum of squares of the distances between each centroid and the global centroid;
 - ratio_ss: the ratio of between_ss and total_ss. This is a measure of how well your data instances can be grouped into clusters.
- Centroids: general statistics for each of the idnetified clusters, including the global one.
- Intercentroid distance: distribution of distances between centroids.

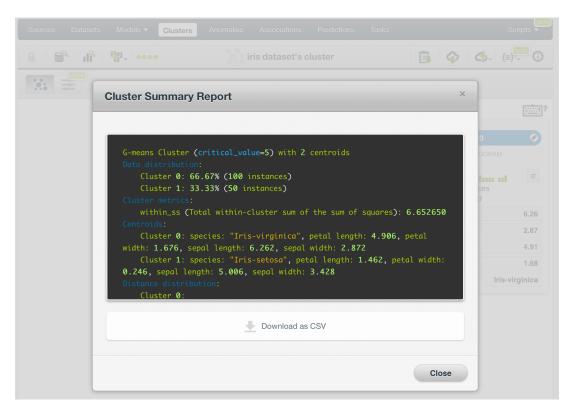


Figure 6.2: Cluster summary report

Cluster Predictions: Centroids

7.1 Introduction

The ultimate goal in building a BigML cluster is being able to make predictions for previously unseen instances with an unknown label. Predictions for clusters are referred to as centroids, since they aim to identify the nearest centroid for new data. In BigML, you can make predictions with clusters based on **single instances** or **multiple instances in batch**. Each **prediction** tells you which is the nearest centroid to your input data along with the distance separating them.

The predictions tab in the main menu of your BigML Dashboard is where all of your saved centroids are listed (see Figure 7.1.)



Figure 7.1: Empty Dashboard centroids view

Cluster predictions are saved under the CLUSTER ANALYSIS option in the menu. (See Figure 7.2.)



Figure 7.2: Menu options of the predictions list view

From this view you can select to view the list for your **single instances centroits** or your **batch centroids** by clicking the corresponding icons. (See Figure 7.3 and Figure 7.4.)



Figure 7.3: Single predictions icon



Figure 7.4: Batch predictions icon

In the predictions list view, you can see, for each prediction, the **Cluster** icon used for the prediction, the **Name** of the prediction, the nearest **Centroid** predicted, the **Distance** from the specified input data, and the **Age** (time since the prediction was created). You can also search your predictions by name by clicking the SEARCH icon on the top right menu in Figure 7.1.

By default, when you first create an account at BigML, or every time that you start a new project, your list view for predictions will be empty. (See Figure 7.5.)

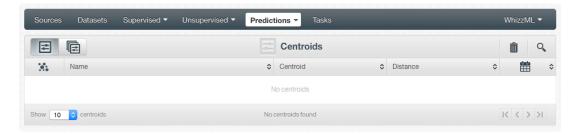


Figure 7.5: Empty Dashboard centroids view

Centroids are saved under the **cluster icon** in the menu options on the top left corner of the **predictions** list view.

7.2 Predicting Centroids

As shown in Figure 7.6, BigML provides two options to create centroids from your cluster:

- CENTROID: to predict single instances.
- BATCH CENTROID: to predict multiple instances in batch.



Figure 7.6: Centroid option from cluster pop up menu

7.2.1 Centroid

BigML allows you to quickly find the nearest centroid for single data instances by providing a form containing the fields used by the cluster, so you can easily set the input data and get an immediate response. This option is only available from the BigML Dashboard for clusters with less than 100 fields. If you want to make single instance predictions for clusters with a higher number of fields, you can use the BigML API¹.

Follow the steps detailed below to create a single prediction:

1. Choose the CENTROID option under the cluster **1-click menu** (see Figure 7.7).

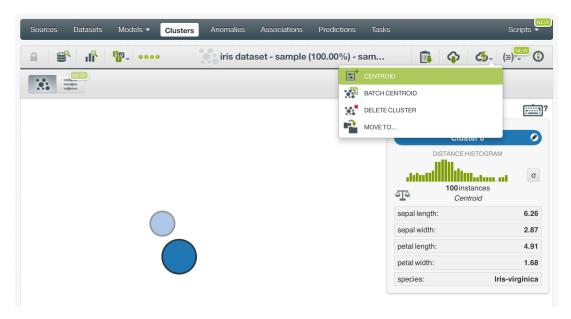


Figure 7.7: Predict option from cluster 1-click menu

Alternatively, click the CENTROID option in the pop up menu in the list view as shown in Figure 7.6.

2. You will be redirected to the **prediction form** where you will find all the fields used by the cluster.

¹ https://bigml.com/api/centroids

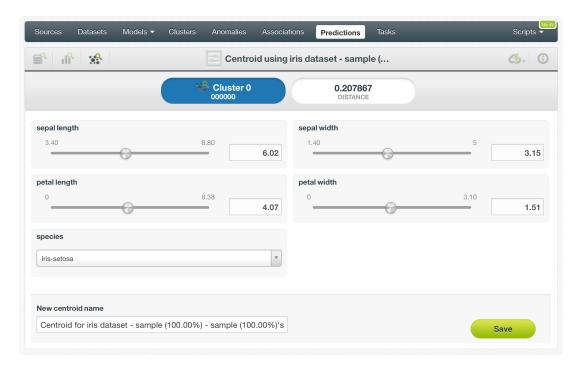


Figure 7.8: Single predictions form

- 3. **Set input values** for the cluster fields. Depending on the field type, you will need to input the values differently:
 - Numeric fields: move the slider or input a specific value in the edition box.
 - · Categorical fields: select one class from the selector.
 - Text fields: write one or several terms in the free text box.
 - Date-time fields: select the appropriate values from the selector.
 - Items fields: when you write the first three characters of an item name, several items matching those characters will appear, so you can select the right one. You can input more than one item for a field.
- 4. **Get the centroids** along with the **distance** displayed on the top of the form. BigML predictions are synchronous, i.e., when you send the input data you get an immediate response. Moreover, single centroids are calculated locally so when you configure the input data you can see how predictions change immediately. (Read more about local predictions in Figure 7.2.1).

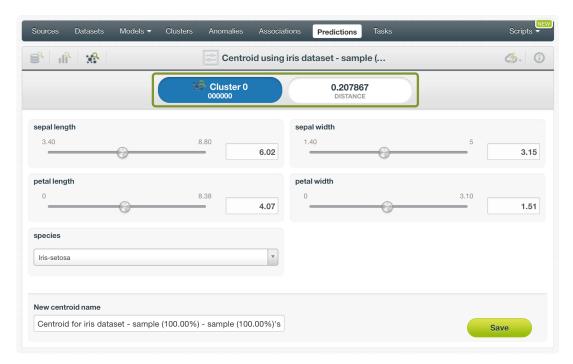


Figure 7.9: Single predictions view

5. Optionally, Save the prediction so you can get a view of the single clusters predictions (see Subsection 7.4.1) and also to find it afterwards in the prediction list view.

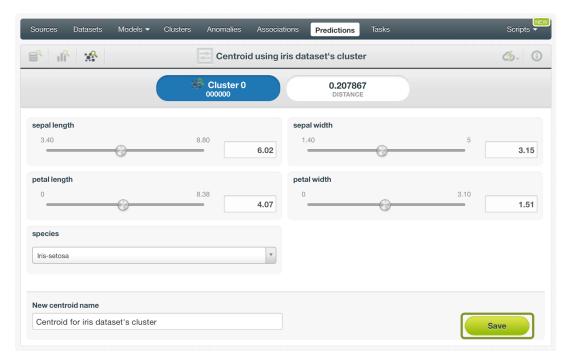


Figure 7.10: Save single cluster predictions

Local Predictions

BigML provides local predictions from the BigML Dashboard for single instance predictions. Local predictions allow you to get a real-time prediction without consuming any credits or requiring an internet connection. This is possible because your cluster is **saved in the browser's memory** so when the input values change, BigML immediately calculates the nearest centroid in a matter of microseconds.

Centroid with Images

BigML clusters can be trained from images using extracted image features (Section 2.4). Because image features are automatically generated numeric fields, creating centroids with images is the same as creating other centroids. The only thing different is input fields of images.

Note: When the input fields contain images, in order to create the centroid, BigML will extract image features automatically to match what were used in the dataset to train the cluster.

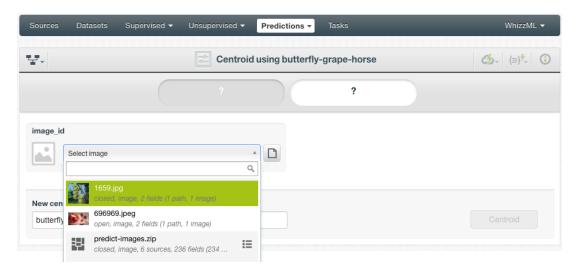


Figure 7.11: Select a single image source in the image input field

The cluster in Figure 7.11, "butterfly-grape-horse", was created from a dataset containing image features extracted from a pre-trained CNN, *ResNet-18*. Creating a centroid using the cluster will be directed to the **prediction form** which presents all input fields used by the cluster. One of them is the image field. Because this is a single centroid, which is a single prediction, an image is input by using a single image source. Clicking on the input field box, single image sources available will be in the dropdown list. There is also a search box which can be used to locate specific ones.

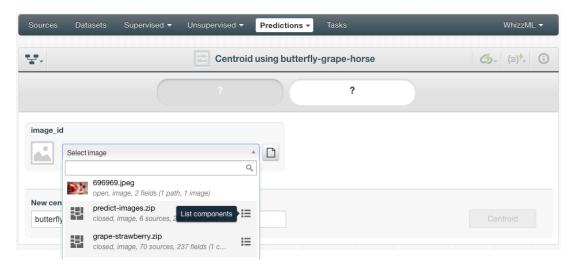


Figure 7.12: List the components of a composite source

Oftentimes single image sources were used for creating a composite source, they become component sources of the composite source. Or an image was uploaded as a part of an archive file (zip/tar) which created a composite source. In those cases, the composite source will be shown in the dropdown list, along with an icon "List components". In the example in Figure 7.12, predict-images.zip is a composite source, click on the icon to show its component sources.

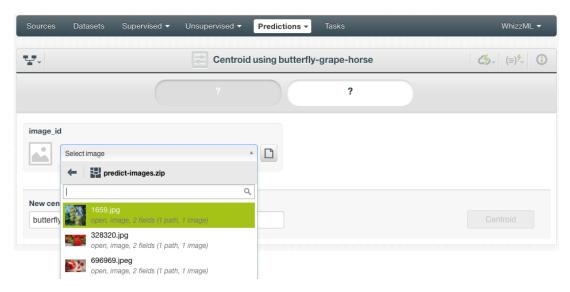


Figure 7.13: Select a component of a composite source

After the component sources of the composite are listed, scroll the dropdown list to find the desired one, then click to select it, as shown in Figure 7.13. There is also a search box to locate specific component sources.

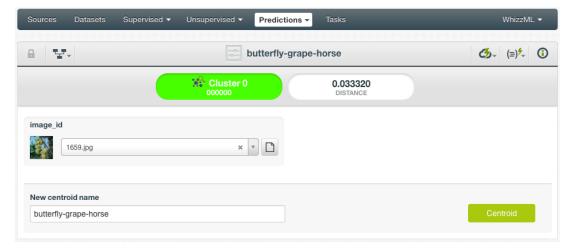


Figure 7.14: A centroid with images

After a new centroid is created, as shown in Figure 7.14, the predicted cluster is at the top of the form along with its distance. The centroid interface is the same as ones created by non-image clusters. Everything described earlier in this section (Subsection 7.2.1) applies.

7.2.2 Batch Centroid

BigML batch centroids allow you to make predictions for multiple instances simultaneously. All you need is the cluster you want to use to make predictions and a dataset containing the instances for which you want to calculate the nearest centroids. BigML will create a prediction for each instance in the dataset. Follow the steps detailed below to create a batch centroid:

1. Select the BATCH CENTROID option under the cluster 1-click menu (see Figure 7.15) or the CREATE BATCH CENTROID option from the pop up menu of the list view (see Figure 7.15).

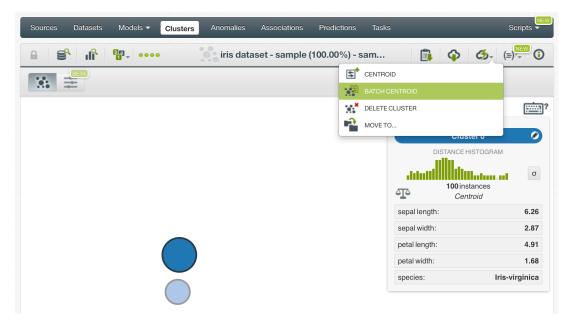


Figure 7.15: Batch centroid option from cluster 1-click menu



Figure 7.16: Batch centroid option from cluster pop up menu

- 2. **Select the dataset** containing all the instances you want to predict. The instances should contain the input values for all the fields used by the cluster. Remember that BigML batch centroids can handle missing data in your prediction dataset only for categorical, text and items fields but not for numeric fields (see Section 4.4). Instances with missing data for numeric fields will be ignored.
- 3. **Optionally, select the cluster** you want to use for the prediction. BigML pre-selects the cluster you created the batch centroid from at step 1, but you can change it at any time in the batch centroid view by selecting another cluster from the custer selector displayed in the right pane.

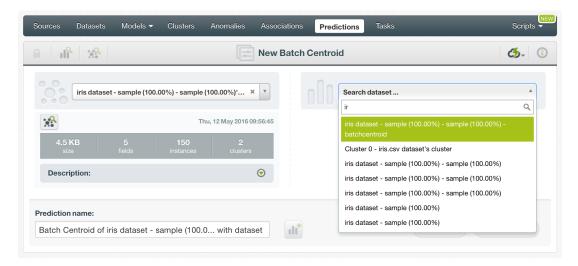


Figure 7.17: Select dataset for batch predictions

4. Once the cluster and the dataset are selected, the batch centroid **configuration options** will appear along with a **preview of the prediction output** (a CSV file). The default format includes all your cluster fields and adds a last column with the cluster predictions.

Note: BigML does not include by default the calculated distance from the centroid, so you will have to configure your output file to include that information. You can find a detailed explanation of all configuration options in Section 7.3.

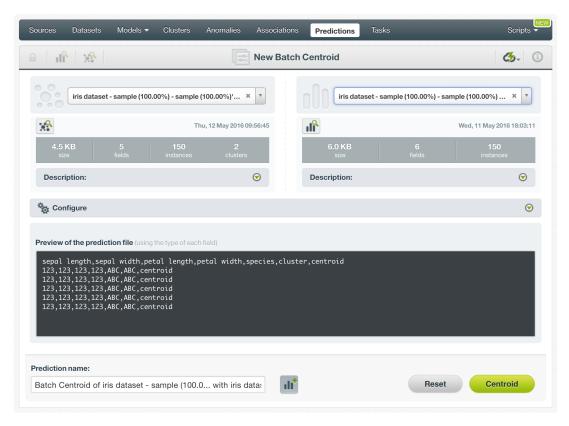


Figure 7.18: Configuration options displayed and output preview

5. By default, BigML generates an output dataset with your batch centroids that you can later find in your datasets section in the BigML Dashboard. This dataset can be helpful to analyze your results afterwards. This option is active by default, but you can deactivate it by clicking in the icon shown in Figure 7.19

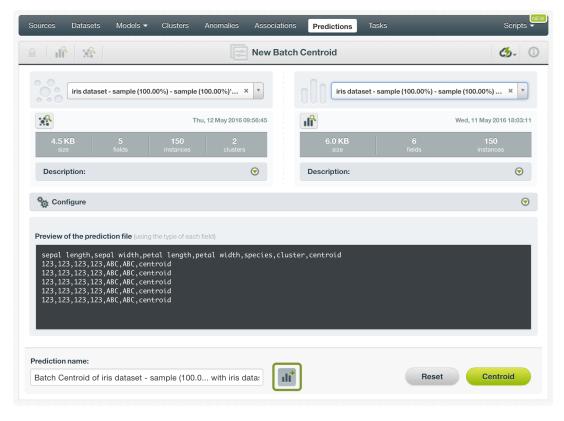


Figure 7.19: Create dataset from batch predictions

6. Once you have your batch centroid configured, click in the green Centroid button to generate your batch prediction.

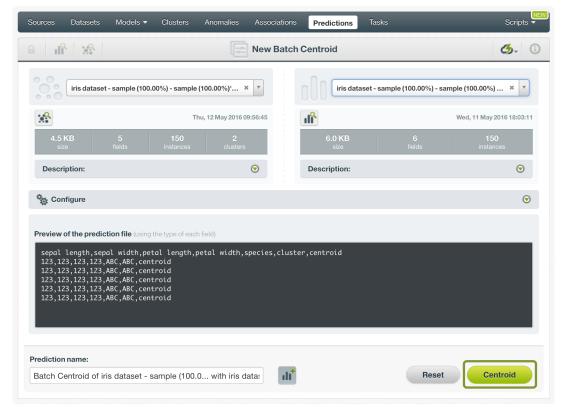


Figure 7.20: Predicting batch centroids

7. When the batch centroid is created, you will be able to **download the CSV file** containing all your dataset instances along with a prediction for each one of them. (See Figure 7.21).

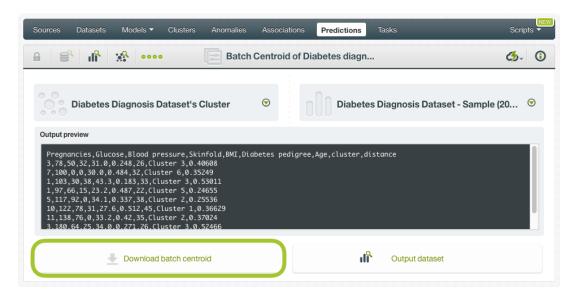


Figure 7.21: Download batch centroid output CSV file

8. If you didn't disable the option to create a dataset, explained in step 4, you will also be able to access the **output dataset** from the batch centroid view.

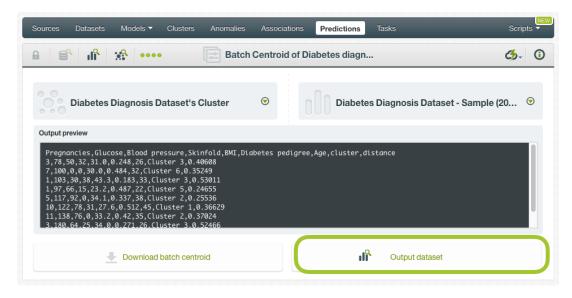


Figure 7.22: View batch predictions output dataset

Batch Centroid with Images

BigML clusters can be trained from images using extracted image features (Section 2.4). The input of a batch centroid is a dataset. So when creating a batch centroid with images, the dataset has to have the same image features used to train the cluster. The image features are in the dataset used to create the cluster.

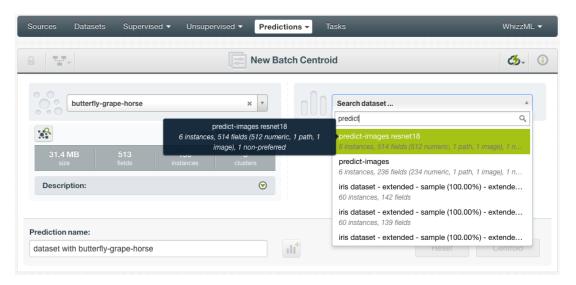


Figure 7.23: Batch centroid using an image dataset

As shown in Figure 7.23, the input for the batch centroid is selected as predict-images resnet18, which is a dataset consisting of six images and contains image features extracted from a pre-trained CNN, *ResNet-18*.

Image features are configured at the source level. For more information about the image features and how to configure them, please refer to section Image Analysis of the Sources with the BigML Dashboard²[6].

For the rest of batch centroids with images, including batch centroid configuration options and output datasets, everything stated earlier in current section (Subsection 7.2.2) applies.

7.3 Configuring Centroid Predictions

BigML provides several options to configure your centroids, such as defining the automatic **fields mapping** performed by BigML (Subsection 7.3.1) and the **output file settings** (Subsection 7.3.2)

7.3.1 Field Mapping

By default, BigML maps fields based on their **names**. If there is a mismatch between the field names in your cluster and those in the input dataset you selected for the batch centroid, you can specify the right correspondence between the two sets of fields by explicitly assigning to each field appearing in the "Cluster fields" column its associated input field in the "Dataset fields" column. (See Figure 7.24.)

If the dataset's and cluster's field names do not match but their IDs do, which happens when corresponding fields appear in the same order, you can tell BigML to use the **field ID** instead of the field name to map the fields. To this aim, click the green switcher shown in Figure 7.24.

If you do not want some of the fields to be considered during the evaluation, you can also **manually** search for those fields and remove them from the "Dataset fields" column.

²https://static.bigml.com/pdf/BigML_Sources.pdf

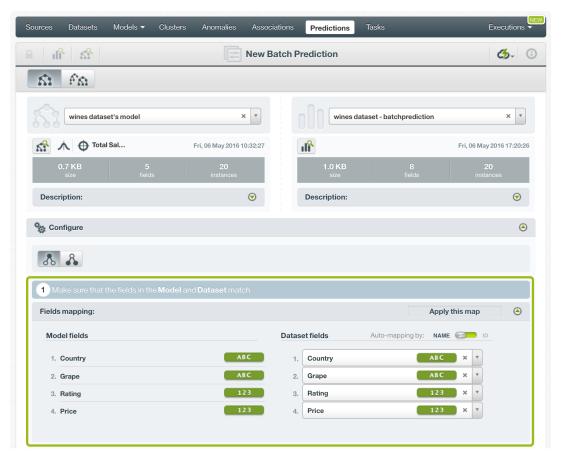


Figure 7.24: Field Mapping for batch centroids

The field mapping from the BigML Dashboard has a **limit of 200 fields**. For batch centroids with higher number of fields, use the argument field_map from BigML API³ if you need to map your fields.

7.3.2 Output Settings

As mentioned, batch centroids can return a CSV file containing all input instances along with the predictions BigML calculated for each of them. Define the following settings to customize your output file:

- **Separator**: this option allows you to choose a separator for your output file values. The default separator is the comma. You can also select the semicolon, the tab, or the space.
- **New line**: this option allows you to set the new line character to use as the line break in the generated csv file: "LF", "CRLF".
- Output fields: this option allows you to include or exclude any of your dataset fields from the output file from the preview shown in Figure 7.25.

Note: a maximum of 100 fields are displayed in the preview, but all your dataset fields are included in the output file by default unless you exclude them.

- **Headers**: this option includes or excludes a first row in the output file (and in the output dataset) with the names of each column. By default, BigML includes the headers..
- **Distance**: this option allows you to include an additional column in the output file with the distance between the instance and the centroid. By default, BigML does not include this column.
- **Centroid column name**: this option allows you to customize the name for the distance column. By default BigML uses "distance".

 $^{^{3} \}texttt{https://bigml.com/api/batchcentroids\#bp_batch_centroid_arguments}$

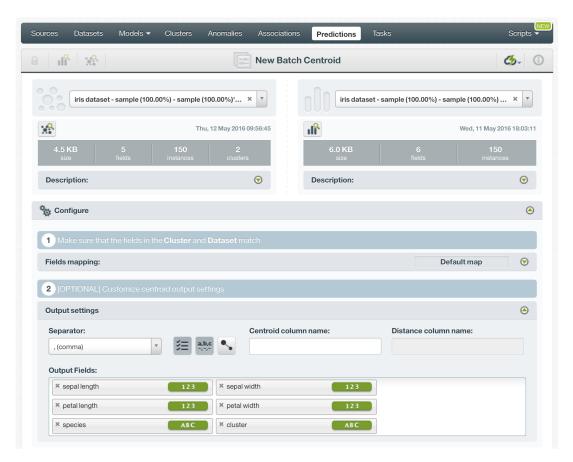


Figure 7.25: Output settings for batch centroids

7.4 Visualizing Cluster Predictions

Centroid visualization changes depending on whether you are predicting one **single** instance CENTROID or multiple instances using the BATCH CENTROID option (see Subsection 7.4.1).

7.4.1 Single Centroid

For single instance predictions, you can find the nearest centroid at the top of the form along with its distance from the input data. (See Figure 7.26.) You can change the value of the displayed input fields any time to have your prediction recalculated in real time.

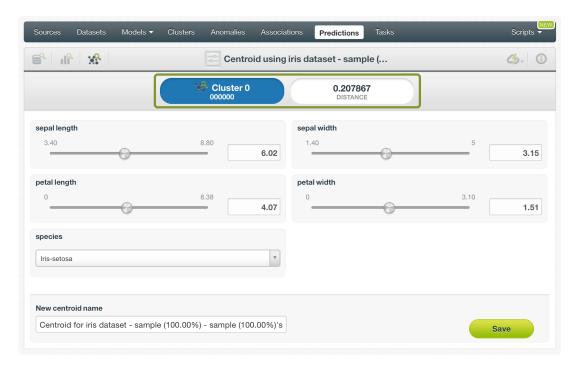


Figure 7.26: Single predictions view

7.4.2 Batch Predictions

For batch centroids, you always get a CSV file and an optional output dataset.

Output CSV File

From the batch centroid view, you can access the CSV file containing your **predictions** for each of your dataset instances in the last column (see Figure 7.27.)

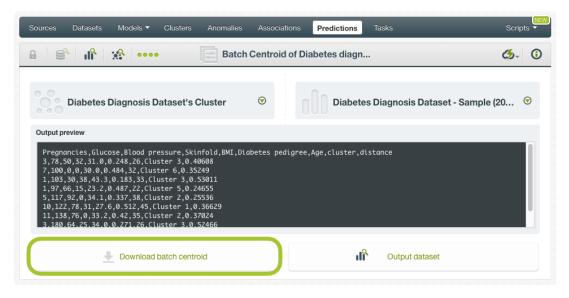


Figure 7.27: Download batch centroid output CSV file

You can configure several options to **customize your CSV file** including the separator for the columns, the name of your centroid and distance column, the dataset fields you want to include, and whether you want to include the headers for your fields. You can find a detailed explanation of those options in Subsection 7.3.2.

Note: by default, BigML does not include the centroid distance in your output file. Click the relevant option from the output settings panel if you want to include it.

See an output CSV file example in Figure 7.28 where the two last columns contain the cluster and the distance for each instance.

```
Pregnancies, Glucose, Blood pressure, BMI, Age, cluster, distance

3,78,50,32,26, Cluster 3,0.40608

7,100,0,0,30,32, Cluster 6,0.35249 1,103,30,38,33, Cluster 3,0.53011

1,97,66,15,17,22, Cluster 5,0.24655 5,117,92,0,38, Cluster 2,0.25536

10,122,78,31,45, Cluster 1,0.36629 11,138,76,0,35, Cluster 2,0.37024

3,180,64,25,26, Cluster 3,0.52466 7,133,84,0,37, Cluster 2,0.36563
```

Figure 7.28: An example of a batch centroid CSV file

Output Dataset

By default BigML automatically creates a dataset out of your batch centroid. (See Subsection 7.3.2.) You can access your output dataset from the batch centroid view as shown in Figure 7.30.

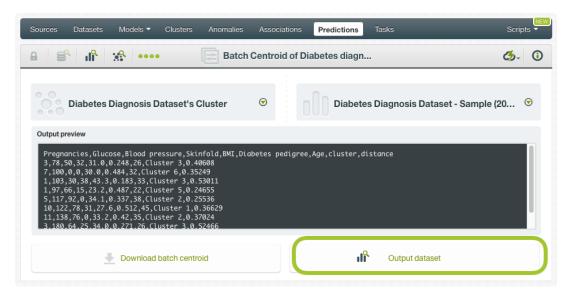


Figure 7.29: View batch centroid output dataset

In the output dataset you can find an additional **field** (named by default "cluster") containing the nearest **centroid** for each one of your instances. If you configured your batch centroid to include the **distance** you will be able to find it in the last field of your output dataset as shown in Figure 7.30.

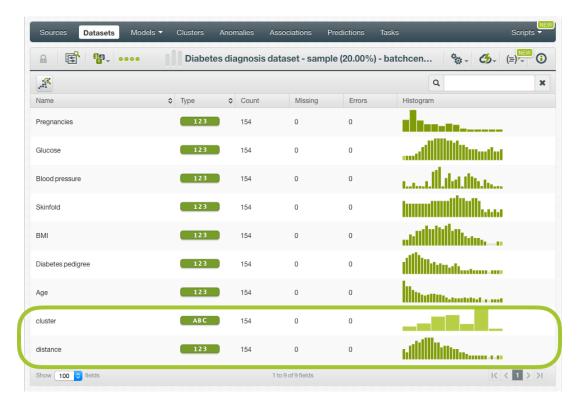


Figure 7.30: Batch centroid output dataset

Batch Centroid 1-Click Actions

From the batch centroid view you can perform the following actions shown in Figure 7.31

- BATCH CENTROID AGAIN: this option will redirect you to the batch centroid creation view where you will have the same cluster and prediction dataset already selected. This option will rapidly create the batch centroid using a different configuration.
- BATCH CENTROID WITH ANOTHER DATASET: this option is an easy way to create a batch centroid using the same cluster and a different dataset.
- BATCH CENTROID USING ANOTHER CLUSTER: this option will easily create a batch centroid using the same dataset and a different cluster.
- NEW BATCH CENTROID: this option will redirect you to the batch centroid creation view where you can select a prediction dataset and a cluster to create your batch centroid.

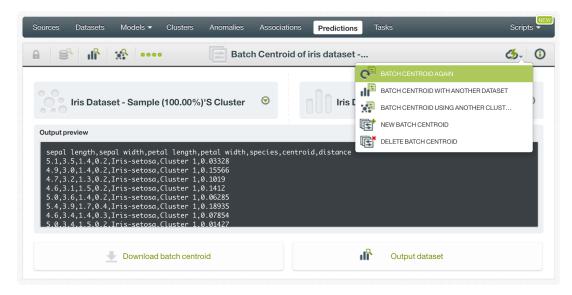


Figure 7.31: Batch centroid 1-click actions

7.5 Consuming BigML Centroids Programmatically

BigML provides plenty of means for developers to integrate BigML centroids within their apps. In the following sections, we will describe how you can use BigML REST API and BigML Python bindings to work with centroids.

7.5.1 Using Centroids Via the BigML API

Centroids have full citizenship in the BigML API. This means you can programmatically create, update, list, and delete them. For example, this is how you can create a single centroid using the command line from a given cluster and defining the input data. This will require properly setting the BIGML_AUTH environment variable to contain your authentication credentials:

For more information on using centroids through the BigML API, please refer to centroid REST API documentation.

7.5.2 Using Centroids Via BigML Bindings

BigML bindings provide a convenient way to access BigML REST API from your language of choice. They offer a higher-level view of BigML Machine Learning resources and algorithms in a number of languages, including Python, Node.js, Java, Swift, and Objective-C. For example, this is how you can create a centroid in Python using BigML bindings:

BigML bindings also provide the means to calculate the nearest centroid locally, without ever hitting the network, which can greatly improve the latency of predicting from your apps. This is made possible by BigML clusters being white-box, meaning you can download and use them independently from BigML. For example, the following code snippet shows how you can download a cluster and use it for making a local prediction using BigML bindings for Python:

For more information on using centroids through the BigML API, please refer to BigML bindings documentation.

7.6 Descriptive Information

Descriptive information is what allows you to describe a centroid so you can find it later and easily recognize it among other centroids.

Each centroid has an associated **name**, **description**, **category**, and **tags**. You can find a brief description for each concept in the following subsections. In Figure 7.32, you can see the options that the **More info** panel gives to edit them.

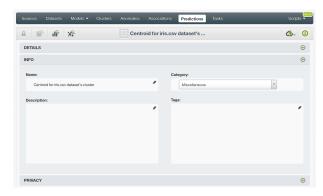


Figure 7.32: Edit centroids

7.6.1 Name

If you do not specify a **name** for your predictions, BigML assigns a default name depending on the type of predictions:

- Single centroid: the name always follows the structure "Centroid for <objective field name>".
- Batch centroid: BigML combines your prediction dataset name and the cluster name: "Batch centroid for <cluster name> with <dataset name>".

Centroid names are displayed in the list view and also on the top bar of a prediction view. Centroid names are indexed to be used in searches. You can rename your centroids at any time from the **More info** panel.

The name of a centroid cannot be longer than 256 characters. There is no restriction on the characters that can be used in a name. More than one centroids can have the same name even within the same project, since they are automatically assigned unique internal identifiers.

7.6.2 Description

Each cluster prediction also has a **description** that it is very useful for documenting your Machine Learning projects. Centroids take the description from the clusters used to create them.

Descriptions can be written using plain text and also markdown⁴. BigML provides a simple markdown editor that accepts a subset of markdown syntax. (See Figure 7.33.)



Figure 7.33: Markdown editor for centroids descriptions

Descriptions cannot be longer than 8192 characters and can use almost any character.

7.6.3 Category

Each prediction has associated a **category** taken from cluster used to create it. Categories are useful to classify predictions according to the domain which your data comes from. This is useful when you use BigML to solve problems across industries or multiple customers.

A prediction category must be one of the categories listed on table Table 7.1.

⁴https://en.wikipedia.org/wiki/Markdown

Category Aerospace and Defense Automotive, Engineering and Manufacturing

Table 7.1: Categories used to classify predictions by BigML

Banking and Finance Chemical and Pharmaceutical Consumer and Retail Demographics and Surveys Energy, Oil and Gas Fraud and Crime Healthcare Higher Education and Scientific Research Human Resources and Psychology Insurance Law and Order Media, Marketing and Advertising Miscellaneous Physical, Earth and Life Sciences **Professional Services** Public Sector and Nonprofit Sports and Games **Technology and Communications** Transportation and Logistics Travel and Leisure Uncategorized Utilities

7.6.4 Tags

A prediction can also have a number of tags associated with it that can help to retrieve it via the BigML API or to provide predictions with some extra information. Your prediction inherits the tags from the cluster use to create it. Each tag is limited to a maximum of 128 characters. Each prediction can have up to 32 different tags.

7.7 **Cluster Predictions Privacy**

The link displayed in the **privacy** panel is the private URL of your centroid, so only a user logged into your account is able to see it. Neither single nor batch centroids can be shared from your BigML Dashboard by sharing a link, as you can do with other resources.



Figure 7.34: Private link of a prediction

7.8 Moving Centroids

When you create a cluster prediction, it will be assigned to the same **project** where the original cluster is located. You cannot move predictions between projects as you do with other resources.

7.9 Stopping Centroids

Single centroids are synchronous resources, so you cannot cancel them during the creation since you get the result immediately.

Batch centroids are asynchronous resources, so you can stop the creation before the task is finished. You can use the DELETE option from the 1-click action menu (Figure 7.35) or from the pop up menu on the clusters list view. If you stop the prediction during its creation, you won't be able to resume the same task again, so if you want to create the same prediction, you will have to start a new task.

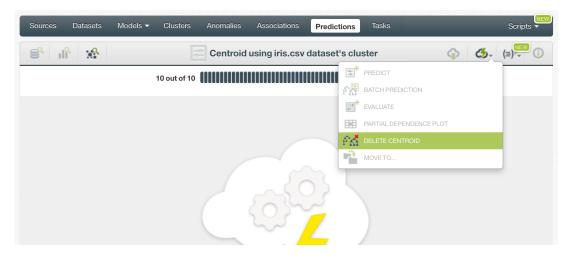


Figure 7.35: Stop prediction from the 1-click menu

7.10 Deleting Centroids

You can DELETE your **single or batch centroids** from the predictions view, using the 1-click action menu (see Figure 7.36) or using the pop up menu on the predictions list view (see Figure 7.37).

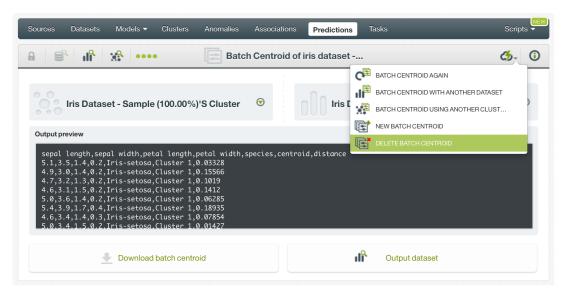


Figure 7.36: Delete prediction from the 1-click menu



Figure 7.37: Delete prediction from popu up menu

A modal window will be displayed asking you for confirmation. Once a prediction is deleted, it is permanently deleted and there is no way you (or even the IT folks at BigML) can retrieve it.

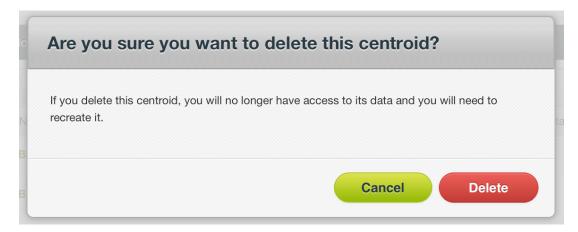


Figure 7.38: Delete prediction confirmation

Consuming Clusters

In the previous sections, we have described how you can create clusters, configure them, use them to make predictions, and more. This section will introduce a number of BigML features that enable powerful ways of taking advantages of BigML clusters: exporting them locally, and using them programmatically via the BigML REST API and BigML Python bindings.

8.1 Exporting and Downloading Clusters

You can download your cluster in several languages including Python, JSON PML or Node.js. Click on the downloading icon in the top menu, and select your preferred language.

By downloading your cluster, you will be able to compute centroids locally, free of latency and at no cost. It works the same way as local predictions for clusters and ensembles.

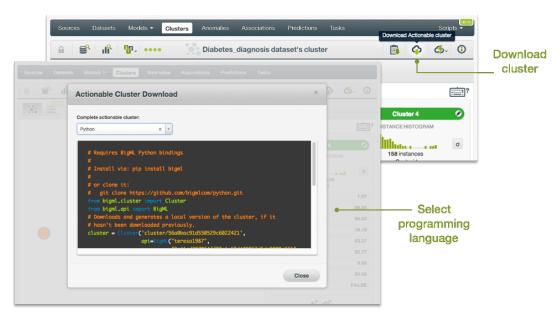


Figure 8.1: Download your cluster

8.2 Updating Clusters

Change the names of your individual clusters by clicking on the edit icon next to each cluster's name.



Figure 8.2: Edit a cluster name

8.3 Using Clusters Via the BigML API

Clusters have full citizenship in the BigML API. This means you can programmatically create, update, list, delete, and use them for predictions. For example, this is how you can create a cluster from the command line with custom values for a few available arguments. This will require you have properly set the BIGML_AUTH environment variable to contain your authentication credentials:

For more information on using clusters through the BigML API, please refer to cluster REST API documentation.

8.4 Using Clusters Via the BigML Bindings

BigML bindings provide a convenient way to access the BigML REST API from your language of choice. They offer a higher-level view of BigML Machine Learning resources and algorithms in a number of languages, including Python, Node.js, Java, Swift, and Objective-C. For example, this is how you can create a cluster in Python using BigML bindings:

For more information on using clusters through the BigML API, please refer to BigML bindings documentation.

Clusters Limits

BigML imposes a few limits to the characteristics of a cluster:

- K-means: BigML K-means can handle up to 300 cluster groups.
- G-means: BigML G-means can handle up to 128 cluster groups.
- **Histogram & planets**: You can use the histogram & planets visualization for clusters if your dataset contains less than 8 numeric fields and no other categorical or text data.

Cluster Descriptive Information

Each cluster has an associated **name**, **description**, **category**, and **tags**. A brief description follows for each concept. In Figure 10.1, you can see the options the **More info** panel provides to edit them.

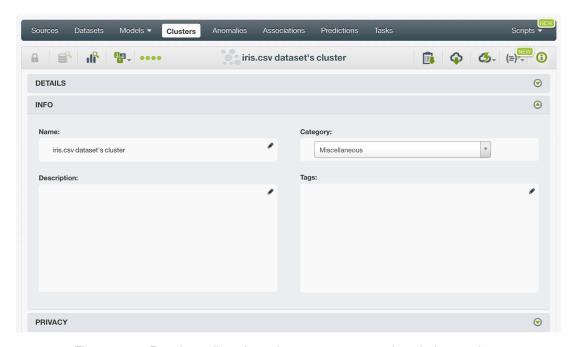


Figure 10.1: Panel to edit a cluster's name, category, description, and tags

10.1 Cluster Name

Each cluster has an associated **name** that is displayed on the list view and also on the top bar of a cluster view. Cluster names are indexed to be used in searches. When you create a cluster, by default, it gets the name of the dataset that you used to create it. You can edit it using the MORE INFO menu option on the right corner of the cluster view (see Figure 10.1). The name of a cluster cannot be longer than **256** characters. There is no restriction on the characters that can be used in a cluster name. More than one cluster can have the same name even within the same project, since they are automatically assigned unique internal identifiers.

10.2 Description

Each cluster inherits the **description** of the dataset used to create it. Descriptions can be very useful for documenting your Machine Learning projects. Descriptions can be written using plain text and also

markdown¹. BigML provides a simple markdown editor that accepts a subset of markdown syntax. (See Figure 10.2.)

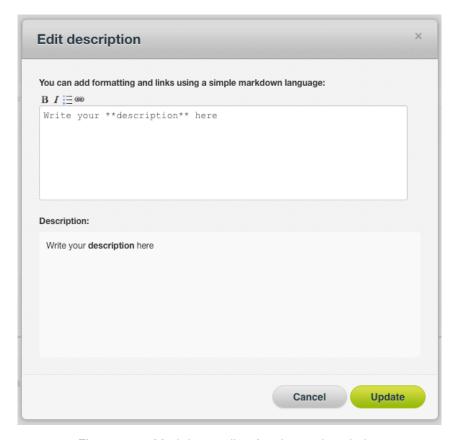


Figure 10.2: Markdown editor for cluster descriptions

Descriptions cannot be longer than 8192 characters and can use almost any character.

10.3 Category

Each cluster takes the category from the dataset used to create it. Categories are useful to classify clusters according to the domain which your data comes from. This is useful when you use BigML to solve problems across industries or multiple customers.

A cluster category must be one of the 24 categories listed in table Table 10.1.

¹ https://en.wikipedia.org/wiki/Markdown

Table 10.1: Categories used to classify clusters by BigML

Category
Aerospace and Defense
Automotive, Engineering and Manufacturing
Banking and Finance
Chemical and Pharmaceutical
Consumer and Retail
Demographics and Surveys
Energy, Oil and Gas
Fraud and Crime
Healthcare
Higher Education and Scientific Research
Human Resources and Psychology
Insurance
Law and Order
Media, Marketing and Advertising
Miscellaneous
Physical, Earth and Life Sciences
Professional Services
Public Sector and Nonprofit
Sports and Games
Technology and Communications
Transportation and Logistics
Travel and Leisure
Uncategorized
Utilities

10.4 Tags

A cluster can also have a number of **tags** associated with it that can help to retrieve it via the BigML API or to provide clusters with some extra information. Clusters inherit the tags of the dataset used to create them.

Each tag is limited to a maximum of 128 characters. Each cluster can have up to 32 different tags.

10.5 Counters

For each cluster, BigML also stores counters to track the number of other resources that have been created using that cluster as a starting point. In the cluster view, you can see a menu option that displays these counters. It also allows you to quickly jump to all the resources of one type that have been created with this cluster as shown in Figure 10.3.



Figure 10.3: Menu option to quickly access to resources created with a cluster

Clusters Privacy

Privacy options for a cluster can be defined in the **More Info** panel, displayed in Figure 11.1. There are two levels of privacy for BigML clusters:

- **Private**: only accessible by authorized users (the owner and those who have been granted access by him or her).
- Shared: by enabling the secret link you will get two different links to share your clusters. The first one is a sharing link that you can copy and send to others so they can visualize and interact with your clusters. The second one is a link to embed your clusters directly on your web page. This is very useful if you want to make local centroid predictions at no cost.

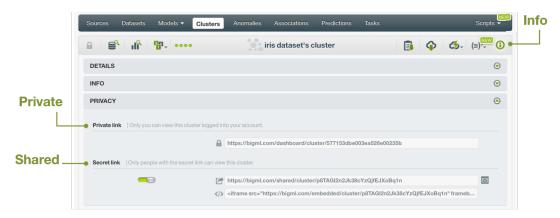


Figure 11.1: Clusters privacy options

Moving Clusters to Another Project

Clusters will be assigned to the same project as the dataset used to create them belongs to. However, you can move clusters between projects. The menu option to do this can be found in two places:

1. In the cluster detail view, among the 1-click actions for each cluster. (See Figure 12.1).

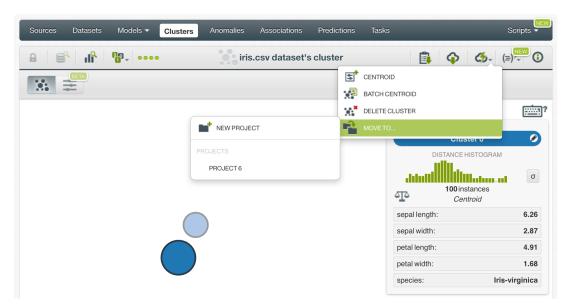


Figure 12.1: Menu option to move clusters

2. In the cluster list view, within the pop up menu (see Figure 12.2).

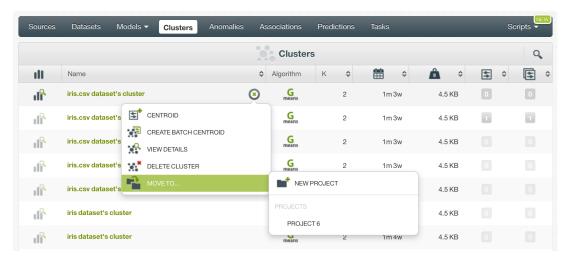


Figure 12.2: Menu option to move clusters from the cluster list view

Stopping Cluster Creation

You can also stop a cluster's creation process, while BigML is not yet done with it, from the 1-click actions menu (Figure 13.1).



Figure 13.1: Menu option to stop a cluster's creation

A modal window (Figure 13.2) will be displayed asking you for confirmation.

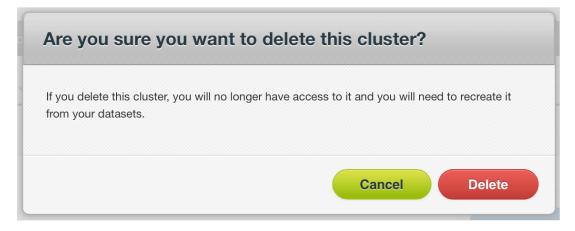


Figure 13.2: Menu option to stop a cluster's creation

Deleting Clusters

You can delete your clusters in two ways:

• From the cluster view, using the 1-click action menu. (See Figure 14.1.)

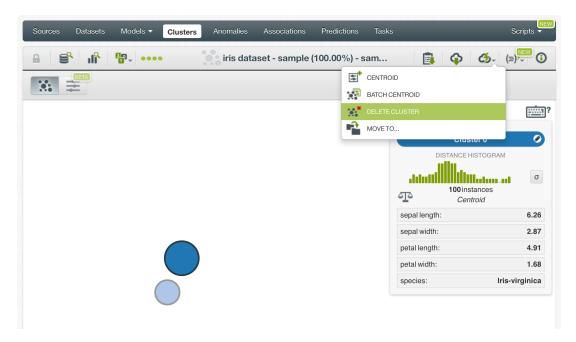


Figure 14.1: Menu option to delete a cluster

• Using the pop up menu on the cluster list. (See Figure 14.2.)



Figure 14.2: Cluster deletion pop up menu option

A modal window (see Figure 14.3) will be displayed asking you for confirmation. Once you delete a cluster, it is deleted permanently and there is no way you (or even the IT folks at BigML) can retrieve it.

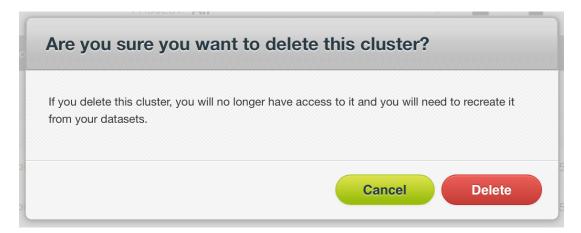


Figure 14.3: Cluster deletion modal window

Takeaways

This document covered clusters in detail. We conclude it with a list of key points:

- BigML Clusters can learn how your data instances group together based on their similarity.
- Each cluster group is represented by its center, called centroid.
- To build a cluster you just need a dataset. (See Figure 15.1).
- A cluster can be an input to a prediction, to a batch prediction, to a dataset, or to a BigML model. (See Figure 15.1).
- Create centroids or batch centroids from a cluster to know to which instance group previously unseen data instances belong.
- You can also create clusters using BigML REST API or the BigML bindings for your language of choice.
- Create a BigML model or a dataset from a cluster to further analyze the instances that belong to any given group of instances discovered by training the cluster. For example, a BigML model may help you identify which fields are more relevant in determining whether a data instance should be considered member of a cluster group.
- Numeric fields are automatically scaled to prevent their different magnitudes from biasing the calculation.
- BigML provides two different methods to do the clustering: K-means and G-means. Use G-means when you do not know how many cluster groups can be found.
- When you create a BigML Cluster from a dataset, you can define a number of options, such as the number K of clusters (K-means) or the critical value (G-means), field scaling and weighting, and sampling.
- BigML visualizes clusters through circles of different colors that represent found centroids. Each circle is sized according to the number of instances that belong to the corresponding cluster group.
- You can use BigML Clusters to calculate the nearest centroid to a given data instance or to a number of instances.
- You can download clusters in several languages, including Python, JSON PML, and Node.js, to use for local computation.
- At any time you can update a cluster's descriptive information, move a cluster to a different project, rename it, or delete it permanently.

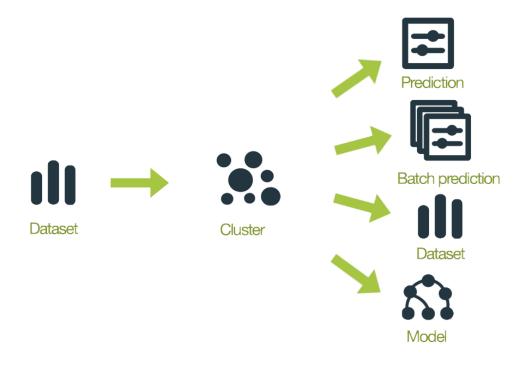


Figure 15.1: Cluster Workflows

Please use the noidx option in the documentclass invocation.

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Glossary

- **Centroids** the center of a cluster found by a clustering algorithm. Centroids are computed by using the mean for numeric fields and the mode for categorical fields. For text and items fields, it selects the values which minimizes the average cosine distance between the centroid and the points in its neighborhood. ii, 1, 27, 62
- Cluster neighborhood the nearest points to the centroid which may finally conform a cluster. 1, 10, 19
- Clustering an unsupervised Machine Learning task in which dataset instances are grouped into geometrically related subsets. ii, 27, 62
- **Dashboard** The BigML web-based interface that helps you privately navigate, visualize, and interact with your modeling resources. ii, 1, 27
- **Dataset** the structured version of a BigML source. It is used as input to build your predictive models. For each field in your dataset a number of basic statistics (min, max, mean, etc.) are parsed and produced as output. ii, 35
- **Field** an attribute of each instance in your data. Also called "feature", "covariate", or "predictor". Each field is associated with a type (numeric, categorical, text, items, or date-time). 1
- **Gaussian distribution** a symmetric probability distribution in which the majority of the mass is clustered about a mean value and values increasingly far from the mean in either direction are increasingly unlikely. Also called the normal distribution or the bell curve. 1
- **G-means** a clustering algorithm that tries to learn the number of different clusters by iteratively taking existing clusters and testing whether the cluster's neighborhood follow a Gaussian distribution. 1
- **Instances** the data points that represent the entity you want to model, also known as observations or examples. They are usually the rows in your data with a value (potentially missing) for each field that describes the entity. ii, 1
- **K-means** the canonical clustering algorithm, which attempts to fit a pre-specified number (*k*) of clusters to the dataset. 1
- **Local predictions** the predictions made in your local environment, faster, at no cost, by downloading your model. 31, 50
- **Missing value** the data points that represent the entity you want to model may present missing value, i.e., not provide a value for all fields that compose the entity. 11
- **Non-preferred fields** fields that, for a number of possible reasons, are by default not included in the modeling process. One example of this is fields that contain the same value for every instance; in general, constant fields add no information to the modeling process. 9

68 Glossary

Predicting the result of obtaining the objective field value for your new data using an existing model. The model returns the predicted value along with a performance measure (confidence for classification or expected error for regression). 27

Predictive Model a machine-learned model that has been created using statistical learning. It can help describe or infer some statistical properties of an entity using the instances provided by a dataset. ii

Project an abstract resource that helps you group related BigML resources together. 2, 28, 57

Sampling the process of partitioning your dataset to consider just a subset of your instances. 14

Unsupervised learning a type of Machine Learning problem in which the objective is not to learn a predictor, and thus does not require each instance to be labeled. Typically, unsupervised learning algorithms infer some summarizing structure over the dataset, such as a clustering or a set of association rules. ii, 1

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