# PCA with the BigML Dashboard 

The BigML Team

Version 1.1

# mi 

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## About this Document

This document provides a comprehensive description of how to reduce your dataset dimensionality using PCA with the BigML Dashboard. Learn how to use the BigML Dashboard to configure, visualize, and interpret this unsupervised model and use it to transform high-dimensional datasets.

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. [3]
- 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:

- Cluster Analysis with the BigML Dashboard. The BigML Team. June 2016. [4]
- Anomaly Detection with the BigML Dashboard. The BigML Team. June 2016. [1]
- Association Discovery with the BigML Dashboard. The BigML Team. June 2016. [2]
- Topic Modeling with the BigML Dashboard. The BigML Team. November 2016. [8]


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## Introduction

Many datasets contain an extremely large number of fields, or highly correlated fields, resulting in suboptimal model performance. Principal component analysis (PCA) is one technique that can be used to transform a dataset in order to yield uncorrelated variables or as a first step in dimensionality reduction. Because PCA transforms the variables in a dataset without accounting for a target variable, it can also be considered an unsupervised Machine Learning method.

The BigML implementation of PCA is distinct from other approaches in that it can handle non-numerical data types, including categorical and text data, as well as combinations of different data types. This allows PCA to be performed on essentially any type of dataset with minimal preprocessing and data cleaning efforts. BigML uses a combination of Principal Component Analysis (PCA) ${ }^{1}$, Multiple Correspondence Analysis (MCA) ${ }^{2}$, and Factorial Analysis of Mixed Data (FAMD) ${ }^{3}$ to deal with different data types. The selection of method is performed automatically without input from the user. The effective difference between the three methods is how the data rows are transformed in order to populate the data matrix. After the matrix is populated, the same decomposition is performed in order to produce the final results.

This document provides a comprehensive description of BigML PCA including how they can be created (Chapter 3) and configured (Chapter 4). Visualizations of the results of a PCA transformation are provided to give insight into the composition of individual principal components and the proportion of variance explained (see Chapter 5). You can use the result of PCA to transform another dataset which contains the same fields, such as datasets resulting from a train/test split (Chapter 6). Finally, it is possible to download and perform PCA either locally or you can create, update, list, and delete PCA resources using the BigML API (Chapter 7).
In BigML, the "Unsupervised" tab of the main menu of your Dashboard allows you to list all of your previously created PCA resources. In the PCA list view (Figure 1.1), you can see, for each PCA resource, the dataset it was created from, as well as the PCA's Name, the number of Components, whether or not it was Standardized, the Age (time elapsed since it was created), Size, and number of batch projections that have been created using that PCA. The SEARCH menu option in the top right corner of the PCA list view allows you to search your PCA resources by name.

[^0]| Sources | Datasets Supervised | Unsupervised | $\text { Predictions } \stackrel{N}{ }$ |  | WhizzM | ML |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\%$ PCAs |  |  |  |  |  |  |
| ill | Name |  |  | 腮 | B ${ }_{\text {B }}$ | 困 |
| Ili | Arrythmia diagnosis <br> 262 components, standardized |  |  | 2d | 536.2 KB | (0) |
| ili | Hotel_reviews standardized |  |  | 6 d 1 h | 1.2 MB | (0) |
| ali | Hotel reviews standardized |  |  | 6d 1n | 1.2 MB | (i) |
| tif | Hotel reviews standardized |  |  | 6d 1h | 24.2 KB |  |
| ali st | Hotel reviews standardized |  |  | 6 d 2 h | 24.2 KB | 18 |
| if | Stumble_upon.csv <br> standardized, default numeric value=mean |  |  | 6 d 2 h | 9.8 MB | (10) |
|  | Stumble_upon.csv felix standardized |  |  | 6d 3h | 9.8 MB | III |
| ili st | Stumble upon with Stumble_upon.csv standardized |  |  | 6d 3h | 10.6 MB | III |
| tio | Fictional Wine Sales <br> standardized, default numeric value=mean |  |  | 6d7h | 50.4 KB | (1i) |
| , if | Fictional Wine Sales standardized |  |  | 6d 8h | 50.4 KB | 1 |
| Show 10 | © pcas |  | 1 to 10 of 17 pcas |  | $1 \ll 12$ | \gg1 |

Figure 1.1: PCA list view

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


Figure 1.2: PCA empty list view in the BigML Dashboard

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


Figure 1.3: PCA icon

## Understanding PCA

This section describes the internal details of BigML principal component analysis (PCA). Beyond a description of the implementation, it also provides information on how to properly make use of PCA in different scenarios, as it can be used as a feature transformation method, a dimensionality reduction technique, and a exploratory data analysis tool.

### 2.1 Principal Component Analysis

Principal component analysis (PCA) is a statistical technique that transforms a dataset defined by possibly correlated variables into a set of uncorrelated variables, called principal components. Each of the principal components is a linear combination of the original variables, is orthogonal ${ }^{1}$ to all other components, and ordered according to the amount of variance explained. PCA preserves the dimensionality of the original dataset and is sensitive to the scaling of the variables in the original dataset.

BigML PCA incorporates multiple factor analysis techniques, rather than only the standard PCA implementation. Specifically, BigML utilizes Multiple Correspondence Analysis (MCA) if the input contains only categorical data and Factorial Analysis of Mixed Data (FAMD) if the input contains both numeric and categorical fields. In the case of items and text fields, data is processed using a bag-of-words approach allowing PCA to be applied. In MCA, categorical variables are first transformed to one-hot ${ }^{2}$ encoded binary vectors. The order of the categorical values matches those found in the field summary. For example, a value of "Iris-virginica" for the "Species" field in the "Iris dataset" becomes [ $0,0,1]$, because "Iris-virginica" is listed third in categories. If the categorical field contains missing values, then an additional element will be appended to the end of this vector to represent missing values. For each categorical value, define a value $p_{j}$ which represents the proportion of the data that contains that value. Continuing with the Iris example, we would have $p_{1}=p_{2}=p_{3}=0.3333$ because the Species values are equally represented in the data. Note that these values are equal to the arithmetic mean of the one-hot encoded columns. In FAMD, numeric fields are transformed identically to PCA. Because of this approach, BigML can handle categorical, text, and items fields in addition to numerical data in an automatic fashion that does not require input by the user.

PCA, MCA, and FAMD all utilize the same decomposition method to yield the final outputs, and differ only in how the data is processed when populating the data matrix.

- PCA: the values for each numeric field are shifted to zero mean, and divided by the standard deviation of the field if standardization is enabled (see Section 4.1).
- MCA: categorical variables are one-hot encoded with an additional field appended to account for missing values. Mean shifted values are divided by the expression $J \times \sqrt{J \times p_{j}}$ where $J$ is the number of categorical fields and $p_{j}$ is the proportion of the data which contains each class.

[^1]- FAMD: numeric fields are transformed identically to PCA and categorical fields are divided by $\sqrt{p_{j}}$.


### 2.2 Missing Values

BigML PCA implementation supports missing values at training and prediction time. To compute a prediction with numeric missing values, the inner product is computed with the missing values set to zero. In the case of missing text or items fields, this is a zero vector the same length as the tag/items cloud. Categorical fields are modeled with an additional categorical value for missing values during model time.

### 2.3 Dimensionality Reduction

While a PCA transformation maintains the dimensions of the original dataset, it is typically applied with the goal of dimensionality reduction. Reducing the dimensions of the feature space is one method to help reduce supervised model overfitting, as there are fewer relationships between variables to consider. Because the principal components yielded by a PCA transformation are linear combinations of the original variables, we are essentially keeping the discriminative aspects of each original variable, even if we reduce the number of dimensions in the new dataset. The principal components yielded by a PCA transformation are ordered by the amount of variance each explains in the original dataset. Plots of the cumulative variance explained, also known as scree plots, are one way to interpret appropriate thresholds for how many of the new features can be eliminated from a dataset while preserving most of the original information (see Chapter 5).

### 2.4 Projections

PCA models can be used to project new data points to the componential axes. This is done by first centering and scaling the input data using the same input transformations as used while modeling, and then taking the inner products between the transformed input and the loading vectors. Note that for text inputs, the centering and scaling are done using the mean and standard deviation computed at model time, as those values are not present in the dataset field summary. Because PCA is a preprocessing technique for many supervised models, it is important to perform the projection on a testing set if PCA is used in the training process.

Projections accept a couple parameters to limit the number of components returned:

- Cumulative variance: a number between $0 \%$ and $100 \%$. The prediction uses the minimum number of components such that the cumulative explained variance is greater than the given threshold. For example, setting a variance threshold of $95 \%$ for the Iris PCA will use only the first two components.
- Maximum components: you can limit the number of components by setting an integer greater than 0 for this parameter.
If no parameters are given, the full set of principal components is used.
Learn more about projections on Chapter 6.


### 2.5 Visualization in the Scatterplot

Appart from the BigML visualization of the PCA components (see Chapter 5), PCA also allow the variance in a dataset to be more easily viewed, as the principal components are ordered by the proportion of variance explained in the original dataset. By performing a batch projection on the original dataset, or another dataset of interest, the resulting dataset can be visualized in the Dashboard using the standard scatterplot ${ }^{3}$. The axes can then be set to the principal components of interest, with PC1 and PC2 being the standard options to view the dimensions that display the greatest variance in the data. For

[^2]supervised problems, the coloration can be set to the target variable in order to visually explore which principal components are maximally discriminative (see Figure 2.1). Because PCA is an unsupervised method and would not include the target variable in the transformation, it is not guaranteed to display separation between classes if the original variables do not contain predictive power.


Figure 2.1: PCA visualization in the scatterplot

## Creating PCA with 1-Click

To create a PCA in BigML you have two options: you can use the 1-click option which uses the default values for all available configuration options, or you can tune the parameters in advance using the configuration option explained in Chapter 4.
You can find the PCA option in the 1-click menu from the dataset view. (See Figure 3.1.)


Figure 3.1: Create PCA from 1-click menu

Alternatively, you can use the PCA option in the pop up menu from the dataset list view. (See Figure 3.2.)


Figure 3.2: Create PCA from popu up menu

Either option builds a PCA using the default values for the available configuration options explained in the following section. (See Chapter 4.)

Note: if you want to use the dataset with the principal components to train supervised models afterward, you will need to exclude the objective field field to create the PCA; otherwise you will be introducing leakage ${ }^{1}$, i.e., the information of the objective field will be contained in the principal components to be used as inputs for your models.

[^3]
## PCA Configuration Options

You can configure a few parameters that affect the way BigML creates PCAs. See the following sections for a detailed explanation.
To display the configuration panel to see all options, click the PCA menu option in the configuration menu from the dataset view. (See Figure 4.1.)


Figure 4.1: Configure PCA

### 4.1 Standardize

The standardize parameter allows you to automatically scale numeric fields to a 0-1 range. If standardize is enabled, the following formula is applied to each numeric field: (field_value - mean)/stddev. Standardizing implies assigning equal importance to all the fields when these are not measured on the same scale. If fields do not have the same scale and you create a PCA with non-standardized fields, it is often the case that each principal component is dominated by a single field. By default, standardization option is enabled.


Figure 4.2: Standardize option for PCA

### 4.2 Default Numeric Value

PCA can include missing values as valid values for any type of fields as explained in Section 2.2. However, there can be situations for which you do not want to include them in your model. For those cases, the Default numeric value parameter is an easy way to replace missing numeric values by another value. You can select to replace them with the field's Mean, Median, Maximum, Minimum or with Zero. (See Figure 4.3.)


Figure 4.3: Select a default value to replace the missing numerics

Note: if your dataset does not contain missing values for your numeric fields, this parameter will not impact your PCA.

### 4.3 Sampling Options

Sometimes you do not need all the data contained in your training dataset to generate your PCA. If you have a very large dataset, sampling may be a good way of getting faster results. (See Figure 4.4.) You can configure the sampling options explained in the following sections.

### 4.3.1 Rate

The rate is the proportion of instances to include in your sample. Set any value between $0 \%$ and $100 \%$. It defaults to 100\%.

### 4.3.2 Range

The range specifies a subset of instances from which to sample, e.g., choose from instance 1 until 200. The Rate you set will be computed over the Range configured.

### 4.3.3 Sampling

By default, BigML selects your instances for the sample by using a random number generator, which means two samples from the same dataset will likely be different even when using the same rates and row ranges. If you choose deterministic sampling, the random-number generator will always use the same seed, thus producing repeatable results. This lets you work with identical samples from the same dataset.

### 4.3.4 Replacement

Sampling with replacement allows a single instance to be selected multiple times. Sampling without replacement ensures that each instance cannot be selected more than once. By default BigML generates samples without replacement.

### 4.3.5 Out of Bag

This argument will create a sample containing only out-of-bag instances for the currently defined rate. If an instance is not selected as part of a sample, it is considered out of bag. Thus, the final, total percentage of instances for your sample will be $100 \%$ minus the rate configured for your sample (when replacement is false). This can be useful for splitting a dataset into training and testing subsets. It is only electable when a sample rate is less than $100 \%$.


Figure 4.4: Sampling options for PCA

### 4.4 Creating PCA with Configured Options

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


Figure 4.5: Create PCA after configuration

### 4.5 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 4.5)). This is to show how to create the PCA programmatically: the endpoint of the REST API call and the JSON that specifies the arguments configured in the panel. Please see (Figure 4.6) below:


Figure 4.6: PCA 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 PCA, 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 PCA

BigML PCA view is composed of two main blocks: PRINCIPAL COMPONENTS (on the left) and SCREE PLOT (on the right). (See Figure 5.1.)


Figure 5.1: PCA view

- PRINCIPAL COMPONENTS is a list containing the principal components calculated by the PCA sorted by variance in descending order. The principal components are named as PCN being $N$ the ranking for each component according to their variance, i.e., PC1 is the first component with the largest variance, PC2 the second most important component and so on. The number of principal components returned should be the same as the number of input fields in the dataset if all the fields are numeric. If the dataset contains categorical, text and/or items fields then you will see a higher number of components since each class, term and item is considered a different field by the PCA (see Chapter 2). You can view up to 200 components in this list (see Figure 5.2).


Figure 5.2: PCA total components

Each principal component includes the following nformation:

- Variance: it indicates how much variability of the data each is explained by each component (see Figure 5.3). It is always a number between $0 \%$ and $100 \%$. The first principal component (PC1) has the largest possible variance and each succeeding component in turn has the highest variance possible under the constraint that it is orthogonal ${ }^{1}$ to the preceding components. All component variances sum up to $100 \%$. If you want to reduce the dimensionality of a given dataset, you should choose the smallest subset of components that explains the largest variance possible to ensure you are not losing dataset information to build other Machine Learning models.

[^4]

Figure 5.3: Principal components variance

- Field weights: below each component you can see a histogram where each bin represents an input field of the original dataset associated with a weight. The weight indicates the influence of each field in a given principal component. This weight can take positive (grey bins) or negative (red bins) values (see Figure 5.4). For categorical, text, or items fields, each class, term and item will have its own weight since they are considered different fields by the PCA.


Figure 5.4: Field weights in components

- The SCREE PLOT is a graphical representation of each principal component (represented by each blue bar on the x-axis) and its variance (represented on the $y$-axis values). The black curve represents the cumulative variance of the components (see Figure 5.5). This visualization helps you to select the subset of components to create a new dataset either by setting a threshold for the cumulative variance or by limiting the total number of components (see slider below the chart in Figure 5.5). Unfortunately, there is not an objective way to decide the optimal number of components for a given cumulative variance. This depends on the data and the problem you are solving. For example, in the Figure 5.5, the first 51 components (which represent less than $20 \%$ of the original 261 dimensions) account for the $80 \%$ of the data variance which seems an acceptably large number to create a new dataset. Moreover, it looks like our dataset confirms the Pareto Principle ${ }^{2}$ which states that $80 \%$ of the effects come from $20 \%$ of the causes, but these results may change depending on the dataset.

[^5]

Figure 5.5: PCA scree plot

By clicking on the icon in the top right of the SCREE PLOT, you can download the chart view in PNG format. (See Figure 5.6.)


Figure 5.6: Export scree plot in PNG format

### 5.1 Create a Dataset From PCA

The final goal of PCA is usually reducing the dataset dimensionality to create other Machine Learning models. This is because lowering the number of fields helps to reduce noise and multicolinearity that may negatively impact the models' performance.

By clicking on the Create dataset button (see Figure 5.7), BigML will create a dataset in your Dashboard. This dataset will contain the principal components taking into account the threshold set using the slider shown in Figure 5.7. By clicking in the icons on the left of the slider, you can choose to either set a threshold for the cumulative variance or limit the number of components. You can also choose to include all or some of the original fields from your dataset by selecting them using the option sown in Figure 5.7. This option is very useful to include ID fields or when your final goal is to build supervised models and you need to include the objective field in the dataset.


Figure 5.7: Create dataset from the PCA view

Behind the scenes, BigML creates a batch projection that you can access from the newly created dataset. If you want to exclude the original fields, tweak any other configuration parameters, or use another dataset, then you can easily do it from the batch projection view as explained in Section 6.3.

## PCA Predictions: Projections

### 6.1 Introduction

You can use your PCA to calculate the principal components for the same data used to create the model or new data that the model has not yet seen. Predictions for PCA are referred to as projections in BigML, since they aim to project the components given a set of values for your instances. PCA is mostly useful to transform all the dataset instances at once and not single instances one at a time. That's why BigML offers only batch projections in the Dashboard and not single projections.

The predictions tab in the main menu of the BigML Dashboard is where all of your saved predictions are listed (Figure 6.1). In the batch projections list view, you can see the icons for the PCA and Dataset used for each projection, the Name of the projection, the Instances used for the projection, and the Age (time since the projection was created). You can also search your projections by name clicking in the search menu option on the top right menu.


Figure 6.1: Projections list view

By default, when you first create an account at BigML, or every time that you start a new project, your list view for projections will be empty. (See Figure 6.2.)


Figure 6.2: Empty Dashboard projections view

Projections are saved under the PCA PROJECTIONS option in the menu (see Figure 6.3.)


Figure 6.3: Menu options of the predictions

The icon shown in Figure 6.4 is the one used for batch projections.


Figure 6.4: Batch projection icon

### 6.2 Creating Projections

BigML usually provides single and batch predictions for most algorithms, i.e., predictions for a single instance or multiple instances simultaneously. However, in the case of PCA, it does not make sense to offer single projections since this model is not useful to predict only one instance at a time.

To create a batch projection in BigML, all you need is the PCA you want to use and a dataset containing the instances for which you want to obtain the principal components.
Follow these steps to create a batch projection:

1. Click on the batch projection option in the PCA 1-click menu. (See Figure 6.5.)


Figure 6.5: Batch projection from 1-click menu

Alternatively, click CREATE BATCH PROJECTION in the pop up menu from the PCA list view as shown in Figure 6.6.


Figure 6.6: Batch projection from pop up menu
2. Select the dataset containing all the instances you want to predict. (See Figure 6.7.) The dataset should contain the input fields used by the PCA to calculate the components. BigML batch projections can handle missing data in your dataset as explained in Chapter 2. From this view you can also select another PCA from the PCA selector.


Figure 6.7: Select dataset for batch projections
3. After you select the PCA and the dataset, the batch projection configuration options will appear along with a preview of the prediction file. (See Figure 6.8.) The default format is a CSV file including all your dataset fields and adding $N$ extra columns for the $N$ components of the PCA. You can configure this file using the output settings explained in Section 6.3.


Figure 6.8: Configuration options displayed and output preview
4. BigML generates an output dataset with your batch projections that you can later find in your datasets section in the BigML Dashboard. This option is active by default, but you can deactivate it by clicking in the icon shown in Figure 6.9.


Figure 6.9: Create dataset from batch projection
5. Finally click on the green Projection button to generate your batch projection.
6. When the batch projection is created, you will be able to download the batch projection containing all your dataset instances along with the PCA components. If you did not disable the option to create a new dataset, you will also be able to access the output dataset from the batch projection view. (See Figure 6.10.)



Figure 6.10: Download batch projection and access output dataset

### 6.3 Configuring Projections

BigML provides several options to configure your projections, such as limiting the number of components (see Subsection 6.3.1), defining the field mapping performed by BigML (see Subsection 6.3.3), and the output file settings (see Subsection 6.3.4).

### 6.3.1 Limit the Number of Components

By default, BigML returns all the principal components in your batch projections. However, you can limit the total number of components to be returned by using either these two options:

- Cumulative variance: you can limit the number of components by setting the maximum data variance that you want them to account for. The right amount of variance depends on the dataset; however, a cumulative variance between $80 \%$ and $90 \%$ is usually enough to avoid losing too much information form the original data.
- Maximum number of components: you can select the exact number of components to be included in the batch projection. This option is useful if you have an ideal number of dimensions that you want to get in the new reduced dataset. Again, the optimal number of components will depend on each specific case.


Figure 6.11: Set a limit for the number of components to be returned

### 6.3.2 Default Numeric Value

For batch projections, the selector to configure the default numeric value to replace the missing values in your dataset will always be disabled. This is because this value needs to be the same as the one used to create the PCA (see Section 4.2). If you did not use any default numeric value to create the PCA, the selector in the batch projection will show a "None" value as you can see in Figure 6.12.


Figure 6.12: See the default nueric value to be used in batch projections

### 6.3.3 Field Mapping

You can specify which fields in the PCA match with which fields in the dataset containing the instances you want to project. BigML automatically matches fields by name, but you can set an automatic match by field ID by clicking in the green switcher shown in Figure 6.13. You can also manually search for fields or remove them if you do not want to consider them during the scoring.


Figure 6.13: Field mapping for batch projections

Note: the field mapping from the BigML Dashboard has a limit of 200 fields. For batch projections with higher number of fields you can use BigML API ${ }^{1}$.

[^6]
### 6.3.4 Output Settings

Batch projections return a CSV file containing all your instances and their scores by default. You can tune the following settings to customize your output file:

- Separator: this option allows you to choose the best separator for your output file columns. The default separator is comma. You can also select semicolon, tab or 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: you have an option to include or exclude all your dataset fields from your output file. You can also select the fields you want to include or exclude one by one from the preview shown in Figure 6.14.
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.


Figure 6.14: Output file settings for batch projections

### 6.4 Visualizing Projections

For batch projections, you always get an output file and, optionally, an output dataset.

## Output File

From the batch projection view you can access the output file preview as shown in Figure 6.15.


Figure 6.15: Download batch projection output file

By default, it will be a CSV file containing all the dataset fields along with all the principal components from the PCA as appended columns. You can customize the output file settings as explained in Subsection 6.3.4.

See an output CSV file example in Figure 6.16 where the last columns contain the components for each instance.

```
Pregnancies,Glucose,Insulin,BMI,PC1,PC2,PC3,PC4
0,137,168,43.1,2.288,3.44,9.76,23.67
11,143,146,36.6,0.254,53.56,2.12,5.76
4,103,192,24.0,0.966,25.7,1.89,5.87
7,106,0,22.7,0.235,2.57,3.65,7.23
2,109,0,42.7,0.845,4.98,3.98,12.45
1,122,220,49.7,0.6.34,1.56,2.78
8,155,495,34.0,28.92,5.98,1.78
4,76,0,34.0,0.391,21.3,3.67,7.34
1,118,94,33.3,0.261,23,1.45,9.45
```

Figure 6.16: An example of a batch prediction CSV file

## Output Dataset

By default, BigML automatically creates a dataset out of your batch projection score. You can disable this option by configuring your batch projection as explained in Section 6.3. You can access your output dataset from the batch projection view as shown in Figure 6.17.


> US Car Accidents
$\odot$
US Car Accidents

Output preview


Figure 6.17: Access batch projection output dataset

In the output dataset you can find $N$ additional fields (named by default "PC $N$ " being " $N$ " an integer starting at 1) containing each of the components from the PCA (see Figure 6.18).


Figure 6.18: Batch projection output dataset

## Batch Projection 1-Click Menu

From the batch projection view you can perform the following actions shown in Figure 6.19

- BATCH PROJECTION AGAIN: this option will redirect you to the batch projection creation view where you will have the same PCA and dataset already selected. It is a quick way if you want to
create the batch projection again using a different configuration.
- BATCH PROJECTION WITH ANOTHER DATASET: this is an easy way to create a batch projection using the same PCA and a different dataset.
- BATCH PROJECTION USING ANOTHER PCA: this is an easy way to create a batch projection using the same dataset and a different PCA.
- NEW BATCH PROJECTION: this will redirect you to the batch projection creation view where you will be able to select a dataset and a PCA to create your batch projection.


Figure 6.19: Batch projection 1-click menu

### 6.5 Consuming Projections

You can fully use batch projections via the BigML API and bindings. The following subsections explain both tools.

### 6.5.1 Using Projections Via the BigML API

You can perform all the projections actions explained in this document such as creating, configuring, retrieving, listing, updating, and deleting projections via the BigML API.
The example below shows how to create a batch projection with after the BIGML_AUTH environment variable that contains your authentication credentials is properly set:

```
curl "https://bigml.io/batchprojection?$BIGML_AUTH" \
    -X POST \
    -H 'content-type: application/json' \
    -d '{"pca": "pca/5423625af0a5ea3eea000028",
        "dataset": "dataset/54222a14f0a5eaaab000000c"}'
```

For more information on using projections through the BigML API, please refer to projections REST API documentation ${ }^{2}$.

### 6.5.2 Using Projections Via the BigML Bindings

You can also create, configure, retrieve, list, update, and delete batch projections via BigML bindings which are libraries aimed to make it easier to use the BigML API from your language of choice. BigML

[^7]offers bindings in multiple languages including Python, Node.js Java, Swift and Objective-C. You can find below an example to create projections with the Python bindings.

```
from bigml.api import BigML
api = BigML()
prediction = api.create_batch_projection("pca/50650bdf3c19201b64000020",
    "dataset/23150b789fdh0175940283")
```

For more information on BigML bindings, please refer to the bindings page ${ }^{3}$.

### 6.6 Descriptive Information

Each projection has an associated name, description, category and tags. Those options are editable through the MORE INFO menu on the top right of the projection view. (See Figure 6.20.)


Figure 6.20: Edit projection metadata from More info panel

### 6.6.1 Projection Name

If you do not specify a name for your scores, BigML assigns a default name by combining your dataset name and the PCA name: "<PCA name> with <dataset name>".

Projection names are displayed on the list view and also on the top bar of a projection view. Projection names are indexed to be used in searches. You can rename your scores at any time from the More INFO menu option.

The name of a projection cannot be longer than 256 characters. More than one projection can have the same name even within the same project, but they will always have different identifiers.

### 6.6.2 Description

Each projection score also has a description that it is very useful for documenting your Machine Learning projects. Single and batch scores take the description from the PCA used to create them.

[^8]Descriptions can be written using plain text and also markdown ${ }^{4}$. BigML provides a simple markdown editor that accepts a subset of markdown syntax. (See Figure 6.21.)


Figure 6.21: Markdown editor for projection descriptions

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

### 6.6.3 Category

Each projection has associated a category. Categories are useful to classify projections according to the domain which your data comes from. This is useful when you use BigML to solve problems across industries or multiple customers. By default, batch projections take the category from the PCA used to create them.

A projection category must be one of the categories listed on Table 6.1.

[^9]Table 6.1: Categories used to classify projections 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 |

### 6.6.4 Tags

A projection can also have a number of tags associated with it that can help to retrieve it via the BigML API or to provide projection with some extra information. Projections inherit the tags from the PCA used to create it.

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

### 6.7 Projection Privacy

The link displayed in the privacy panel is the private URL of your projection, so only a user logged into your account is able to see it. Batch projections cannot be shared from the BigML Dashboard by sharing a link as you can do it with other resources.

| Sources | Datasets | Supervised - | Unsupervised | Predictions - Tasks | WhizzML - |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| (1) 둫 | -0.0 |  | E US car | dents with US car accidents | ¢ (三) $\%$ | (i). |
| details |  |  |  |  |  | $\bigcirc$ |
| info |  |  |  |  |  | $\bigcirc$ |
| PRIVACY |  |  |  |  |  | (1) |
| Private link \|Only you can view this batchprojection logged into your account. |  |  |  |  |  |  |
| A https://strato.dev.bigml.com/dashboard/batchprojection/5c082a87983efc666f0000a6 |  |  |  |  |  |  |

Figure 6.22: Private link of a projection

### 6.8 Moving Projections

When you create a projection it will be assigned to the same project where the original PCA is located. You cannot move projections between projects as you do with other resources.

### 6.9 Stopping Projections Creation

Batch projections are asynchronous resources so you can stop their creation before the task is finished. You can use the DELETE BATCH PROJECTION option from the 1-click menu. (See Figure 6.23.)


Figure 6.23: Stop batch projection from the 1-click menu

Alternatively, you can use the DELETE BATCH PROJECTION from the pop up menu on the projection view. (See Figure 6.24.)


Figure 6.24: Stop batch projection from the pop up menu

Note: if you stop the projection during its creation, you will not be able to resume the same task again. So if you want to create the same projection, you will have to start a new task.

### 6.10 Deleting Projections

You can delete your batch projections by clicking on the DELETE BATCH PROJECTION in the 1-click menu (see Figure 6.25).


Figure 6.25: Delete batch projection from the 1-click menu

Alternatively, you can click the DELETE BATCH PROJECTION in the pop up menu from the projection list view (see Figure 6.26.)


Figure 6.26: Delete batch projection from pop up menu

A modal window will be displayed asking you for confirmation. Once a projection is deleted, it is permanently deleted and there is no way you (or even the IT folks at BigML) can retrieve it. (Figure 6.27.)


Figure 6.27: Delete projection confirmation

## Consuming PCA

Similarly to other models in BigML, you can download PCA and use them locally to make projections. You can also create and consume your PCA programmatically via the BigML API and bindings. The following subsections explain these three options.

### 7.1 Downloading PCA

You can download your PCA in Python. Just click on the DownloAd ACTIONABLE PCA menu option and select your preferred language. (See Figure 7.1.)


Figure 7.1: Downloading PCA

You can predict the principal components for your new data locally, free of latency, and at no cost by downloading your PCA. It works the same way as local predictions for models and ensembles.

### 7.2 Using PCA Via the BigML API

PCAs have full citizenship in the BigML API which allows you to programmatically create, configure, retrieve, list, update, delete, and use them to project new data.
See in the example below how to create a PCA using an existing dataset after you have properly set the BIGML_AUTH environment variable to contain your authentication credentials:

```
curl "https://bigml.io/pca?$BIGML_AUTH"
    -X POST \
    -H 'content-type: application/json' \
    -d '{"dataset": "dataset/50650bdf3c19201b64000322"}'
```

For more information on using PCAs through the BigML API, please refer to PCA REST API documentation ${ }^{1}$.

### 7.3 Using PCA Via the BigML Bindings

You can also create and use PCA via BigML bindings which are libraries aimed to make it easier to use the BigML API from your language of choice. BigML offers bindings in multiple languages including Python, Node.js, Java, Swift and Objective-C. You can find below an example to create a PCA with the Python bindings.

```
from bigml.api import BigML
api = BigML()
pca = api.create_pca('dataset/57506c472275c1666b004b10')
```

For more information on BigML bindings, please refer to the bindings page ${ }^{2}$.

[^10]
## PCA Limits

BigML PCAs have a few limitations regarding the type of input data they can support. BigML also impose some limits on the components to visualize a PCA. You can find all limits listed below:

- Categorical fields: a maximum number of 1,000 distinct classes per field is allowed.
- Text fields: a maximum of 1,000 terms are considered per dataset.
- Item fields: a maximum of 10,000 items are considered per dataset.
- Principal components: a maximum of 200 components are displayed in the PCA view.


## PCA Descriptive Information

PCAs have an associated name, description, category, and tags. The following subsections briefly describe each concept. See in Figure 9.1 the options under More info menu to edit PCAs.


Figure 9.1: Editing PCAs

### 9.1 PCA Name

Each PCA has a name that is displayed in the PCA list view and also on the top bar of the PCA view. PCA names are indexed to be used in searches. When you create a PCA, it gets a default name which is basically the dataset name. You can change it using the MORE INFO menu option on the right corner of the PCA view. The name of a PCA cannot be longer than 256 characters. More than one PCA can have the same name even within the same project, but they will always have different identifiers.

### 9.2 Description

Each PCA also has a description that is very useful for documenting your Machine Learning projects. PCAs take the description of the datasets used to create them by default.

Descriptions can be written using plain text and also markdown ${ }^{1}$. BigML provides a simple markdown editor that accepts a subset of markdown syntax. (See Figure 9.2.)


Figure 9.2: Markdown editor for PCA descriptions

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

### 9.3 Category

A category, taken from the dataset used to create it, is associated with each PCA. Categories are useful to classify PCAs 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 PCA category must be one of the $\mathbf{2 4}$ categories listed in Table 9.1.

[^11]Table 9.1: Categories used to classify PCAs 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 |

### 9.4 Tags

A PCA can also have a number of tags associated with it that can help to retrieve it via the BigML API or to provide PCA with some extra information. PCAs inherit the tags from the dataset used to create them. Each tag is limited to a maximum of 128 characters. Each PCA can have up to $\mathbf{3 2}$ different tags.

### 9.5 Counters

For each PCA, BigML also stores a number of counters to track the number of other resources that have been created using the PCA as a starting point. Display the counters by mousing over the menu option at the top of the PCA view. Click on VIEW \# BATCH PROJECTIONS FROM THIS PCA menu option see all batch projections. (See Figure 9.3.)


Figure 9.3: Counters for PCA

## PCA Privacy

Privacy options for PCA can be defined in the More Info menu option. (See Figure 10.1.) There are two levels of privacy for BigML PCA:

- 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 PCA. The first one is a sharing link that you can copy and send to others so they can visualize and interact with your PCA. The second one is a link to embed your PCA directly on your web page.


Figure 10.1: PCA privacy

## Moving PCA

When you create a PCA, it will be assigned to the same project where the original dataset is located. PCAs can only be assigned to a single project. However, you can move PCAs between projects in your Dashboard or to other Organization projects. The menu option to do this can be found in two places:

1. Click move to... within the 1-click menu from the PCA view. (See Figure 11.1.)


Figure 11.1: Change project from 1-click menu
2. Click move to... within the pop up menu from the PCA list view. (See Figure 11.2)


Figure 11.2: Change project from pop up menu

## Stopping PCA Creation

You can stop the creation of a PCA before the task is finished by clicking the DELETE PCA option in the 1-click menu from the PCA view. (See Figure 12.1.)


Figure 12.1: Stop PCA creation from 1-click menu

Alternatively, click the DELETE PCA in the pop up menu from the PCA list view. (See Figure 12.2.)


Figure 12.2: Stop PCA creation from pop up menu

Note: if you stop the PCA during its creation, you will not be able to resume the same task. If you want to create the same PCA, you will have to start a new task.

## Deleting PCA

You can delete your PCA by clicking the DELETE PCA option in the 1-click menu from the PCA view. (See Figure 13.1.)


Figure 13.1: Delete PCA from 1-click menu

Alternatively, click the DELETE PCA in the pop up menu from the PCA list view. (See Figure 13.2.)


Figure 13.2: Delete PCA from pop up menu

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


Figure 13.3: Confirmation message to delete a PCA

## Takeaways

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

- PCA is an unsupervised learning method used to reduce the dimensionality of your datasets.
- BigML PCA is distinct from other approaches to the PCA algorithm because it lets you transform many different data types in an automatic fashion that does not require you to configure it manually.
- BigML PCA can handle numeric and non-numeric data types, including text, categorical, items fields, as well as combinations of these data types.
- BigML PCA incorporates multiple factor analysis techniques, specifically, Multiple Correspondence Analysis (MCA) if the input contains only categorical data, and Factorial Analysis of Mixed Data (FAMD) if the input contains both numeric and categorical fields
- BigML PCA also supports missing data.
- To create a PCA you just need an existing dataset. Then this PCA model can be used to make a batch projection to calculate the components for any dataset that uses the same input fields as the model. (See Figure 14.1.)
- You can use the 1-click option to create your PCA or you can configure the parameters provided by BigML beforehand.
- When the PCA has been created, you get a list of your PRICNCIPAL COMPONENTS ordered by the amount of data variance they explain.
- You can decide to limit the number of your components to create a new dataset by using the SCREE PLOT.
- You can create a new dataset from the PCA view.
- You can use your PCA to make projections on multiple instances in batch.
- You can create, configure, update, and use your PCA programmatically via the BigML API and bindings.
- You can download your PCA to locally make projections on new instances.
- You can add descriptive information to your PCA.
- You can move your PCA between projects.
- You can share your PCA with other people using the secret link or embedding them into your own applications.
- You can stop your PCA creation by deleting them.
- You can permanently delete your existing PCA.


Figure 14.1: PCA workflow

Please use the noidx option in the documentclass invocation.

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## Glossary

Dashboard The BigML web-based interface that helps you privately navigate, visualize, and interact with your modeling resources. ii

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, 8

Local predictions the predictions made in your local environment, faster, at no cost, by downloading your model. 36

Objective Field the field that a regression or classification model will predict (also known as target). 7
Overfitting the process of tailoring the model to fit the training data at the expense of generalization. 4
PCA Principal Component Analysis is an unsupervised Machine Learning technique used to transform a dataset in order to yield uncorrelated features and reduce dimensionality to build other models. ii, 1, 3, 19
Principal components the set of uncorrelated variables that PCA calculates as linear transformations of the original dataset field values. Each component has a variance associated which indicates the amount of the variability in the data that it captures. $3,4,7,8,12,14,15,17,19,20,24,27$, 36
Project an abstract resource that helps you group related BigML resources together. 2, 19, 44
Projections PCA predictions are called projections in BigML. For PCA, only batch projections are offered in the Dashboard, i.e., projections for multiple instances simultaneously. A batch projection is computed as the inner product of each instance in the components attribute of the PCA and the input vector. 4, 18, 19, 20, 36

Supervised learning a type of Machine Learning problem in which each instance of the data has a label. The label for each instance is provided in the training data, and a supervised Machine Learning algorithm learns a function or model that will predict the label given all other features in the data. The function can then be applied to data unseen during training to predict the label for unlabeled instances. ii, 4

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, 5

Variance (PCA) the variance of each component in PCA means the total variability of the data explained by that component. A higher variance for a given component makes it a better candidate to select as input for other models. 3, 4, 12, 13, 15, 24

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[^0]:    ${ }^{1}$ https://en.wikipedia.org/wiki/Principal_component_analysis
    ${ }^{2} h t t p s: / / e n . w i k i p e d i a . o r g / w i k i / M u l t i p l e \_c o r r e s p o n d e n c e, a n a l y s i s$
    $3^{3}$ https://en.wikipedia.org/wiki/Factor_analysis_of_mixed_data

[^1]:    ${ }^{1}$ https://en.wikipedia.org/wiki/Orthogonality
    ${ }^{2}$ https://en.wikipedia.org/wiki/One-hot

[^2]:    ${ }^{3}$ https://bigml.com/whatsnew\#scatterplot-in-the-dashboard

[^3]:    ${ }^{1}$ https://machinelearningmastery.com/data-leakage-machine-learning/

[^4]:    ${ }^{1}$ https://en.wikipedia.org/wiki/Orthogonality

[^5]:    ${ }^{2}$ https://en.wikipedia.org/wiki/Pareto_principle

[^6]:    ${ }^{1}$ https://bigml.com/api/batchprojections

[^7]:    ${ }^{2}$ https://bigml.com/api/projections

[^8]:    ${ }^{3}$ https://bigml.com/tools/bindings

[^9]:    ${ }^{4}$ https://en.wikipedia.org/wiki/Markdown

[^10]:    ${ }^{1}$ https://bigml.com/api/pca
    ${ }^{2}$ https://bigml.com/tools/bindings

[^11]:    ${ }^{1}$ https://en.wikipedia.org/wiki/Markdown

