cmapBQ

Release 1.0.0

Anup Jonchhe

Dec 16, 2020

CONTENTS

CHAPTER

ONE

INSTALLATION GUIDE

The `cmapBQ` toolkit is available on PyPi and can be installed using: `pip install cmapBQ`

This will install the package into your currently active environment.

From here, ensure you have a Google Service Account Credentials file, documentation can be found at Getting started with authentication

It is recommended to place the credentials in the ~/.cmapBQ folder. To complete installation, run the following command from within a python session. This only needs to be done once, and will populate a ~/.cmapBQ/config.txt file with default table values and correct credentials path.

```
import cmapBQ.query as cmap_query
import cmapBQ.config as cmap_config

cmap_config.setup_credentials(path_to_json)
```

CHAPTER

TWO

GUIDE

- search

2.1 cmapBQ

2.1.1 cmapBQ.config module

class cmapBQ.config.**Configuration**(*credentials: str*, *tables:* cmapBQ.config.TableDirectory)
Data class for configuration of cmapBQ. Object for config.txt

credentials: str

tables: *cmapBQ.config.TableDirectory*

class cmapBQ.config.**TableDirectory**(*compoundinfo: str*, *genetic_pertinfo: str*, *geneinfo: str*, *cellinfo: str*, *instinfo: str*, *siginfo: str*, *level3: str*, *level4: str*, *level5: str*)

cellinfo: str

compoundinfo: str

geneinfo: str

genetic_pertinfo: str

instinfo: str

level3: str

level4: str

level5: str

siginfo: str

cmapBQ.config.**get_bq_client**(*config=None*)
Return authenticated BigQuery client object.

Parameters **config** – optional path to config if not default

Returns BigQuery Client

cmapBQ.config.**get_default_config**()
Get configuration object from reading ~/.cmapBQ/config.txt

Returns cmapBQ.config.Configuration class.

cmapBQ.config.**set_default_config**(*input_config_path*)
Change configuration in ~/.cmapBQ to input config path. Overwrites ~/.cmapBQ/config.txt.,

Parameters **input_config_path** – valid YAML formatted config file

Returns location in ~/.cmapBQ

cmapBQ.config.**setup_credentials**(*path_to_credentials*)
Setup script for pointing config.txt to a GOOGLE_APPLICATION_CREDENTIALS JSON key. Writes default tables if ~/.cmapBQ/config.txt does not exist.

Parameters **path_to_credentials** –

Returns None (side effect)

2.1.2 cmapBQ.query module

cmapBQ.query.**cmap_cell**(*client*, *cell_iname=None*, *cell_alias=None*, *ccle_name=None*, *primary_disease=None*, *cell_lineage=None*, *cell_type=None*, *table=None*, *verbose=False*)
Query cellinfo table

Parameters

- **client** – Bigquery Client
- **cell_iname** – List of cell_inames
- **cell_alias** – List of cell aliases
- **ccle_name** – List of ccle_names
- **primary_disease** – List of primary_diseases
- **cell_lineage** – List of cell_lineages
- **cell_type** – List of cell_types
- **table** – table to query. This by default points to the siginfo table and normally should not be changed.
- **verbose** – Print query and table address.

Returns Pandas DataFrame

cmapBQ.query.**cmap_compounds**(*client*, *pert_id=None*, *cmap_name=None*, *moa=None*, *target=None*, *compound_aliases=None*, *limit=None*, *verbose=False*)
Query compoundinfo table for various field by providing lists of compounds, moa, targets, etc. 'AND' operator used for multiple conditions.

Parameters

- **client** – BigQuery Client
- **pert_id** – List of pert_ids
- **cmap_name** – List of cmap_names
- **target** – List of targets
- **moa** – List of MoAs
- **compound_aliases** – List of compound aliases
- **limit** – Maximum number of rows to return

- **verbose** – Print query and table address.

Returns Pandas Dataframe matching queries

cmapBQ.query.**cmap_genes**(*client*, *gene_id=None*, *gene_symbol=None*, *ensembl_id=None*, *gene_title=None*, *gene_type=None*, *feature_space='landmark'*, *src=None*, *table=None*, *verbose=False*)

Query geneinfo table. Geneinfo contains information about genes including ids, symbols, types, ensembl_ids, etc.

Parameters

- **client** – Bigquery Client
- **gene_id** – list of gene_ids
- **gene_symbol** – list of gene_symbols
- **ensembl_id** – list of ensembl_ids
- **gene_title** – list of gene_titles
- **gene_type** – list of gene_types
- **feature_space** – Common featurespaces to extract. 'rid' overrides selection

  Choices: ['landmark', 'bing', 'aig']

  landmark: 978 landmark genes

  bing: Best-inferred set of 10,174 genes

  aig: All inferred genes including 12,328 genes

  Default is landmark.
- **src** – list of gene sources
- **table** – table to query. This by default points to the siginfo table and normally should not be changed.
- **verbose** – Print query and table address.

Returns Pandas DataFrame

cmapBQ.query.**cmap_genetic_perts**(*client*, *pert_id=None*, *cmap_name=None*, *gene_id=None*, *gene_title=None*, *ensemble_id=None*, *table=None*, *verbose=False*)

Query genetic_pertinfo table

Parameters

- **client** – Bigquery Client
- **pert_id** – List of pert_ids
- **cmap_name** – List of cmap_names
- **gene_id** – List of type INTEGER corresponding to gene_ids
- **gene_title** – List of gene_titles
- **ensemble_id** – List of ensumble_ids
- **table** – table to query. This by default points to the siginfo table and normally should not be changed.
- **verbose** – Print query and table address.

Returns

cmapBQ.query.**cmap_matrix**(*client*, *data_level='level5'*, *feature_space='landmark'*, *rid=None*, *cid=None*, *verbose=False*, *chunk_size=1000*, *table=None*, *limit=4000*)

Query for numerical data for signature-gene level data.

Parameters

- **client** – Bigquery Client
- **data_level** – Data level requested. IDs from siginfo file correspond to 'level5'. Ids from instinfo are available in 'level3' and 'level4'. Choices are ['level5', 'level4', 'level3']
- **rid** – Row ids
- **cid** – Column ids
- **feature_space** – Common featurespaces to extract. 'rid' overrides selection

  Choices: ['landmark', 'bing', 'aig']

  landmark: 978 landmark genes

  bing: Best-inferred set of 10,174 genes

  aig: All inferred genes including 12,328 genes

  Default is landmark.
- **chunk_size** – Runs queries in stages to avoid query character limit. Default 1,000
- **limit** – Soft limit for number of signatures allowed. Default is 4,000.
- **table** – Table address to query. Overrides 'data_level' parameter. Generally should not be used.
- **verbose** – Print query and table address.

Returns GCToo object

cmapBQ.query.**cmap_profiles**(*client*, *sample_id=None*, *pert_id=None*, *pert_type=None*, *cmap_name=None*, *cell_iname=None*, *det_plate=None*, *build_name=None*, *return_fields='priority'*, *limit=None*, *table=None*, *verbose=False*)

Query per sample metadata, corresponds to level 3 and level 4 data, AND operator used for multiple conditions.

Parameters

- **client** – Bigquery client
- **sample_id** – list of sample_ids
- **pert_id** – list of pert_ids
- **pert_type** – list of pert_types. Avoid using only this parameter as the return could be very large.
- **cmap_name** – list of cmap_names
- **det_plate** – list of det_plates
- **build_name** – list of builds
- **return_fields** – ['priority', 'all']
- **limit** – Maximum number of rows to return
- **table** – table to query. This by default points to the siginfo table and normally should not be changed.

- **verbose** – Print query and table address.

Returns Pandas Dataframe

cmapBQ.query.**cmap_sig**(*client*, *sig_id=None*, *pert_id=None*, *pert_type=None*, *cmap_name=None*, *cell_iname=None*, *det_plates=None*, *build_name=None*, *return_fields='priority'*, *limit=None*, *table=None*, *verbose=False*)

Query level 5 metadata table. Multiple parameters are filtered using the 'AND' operator

Parameters

- **client** – Bigquery Client
- **sig_id** – list of sig_ids
- **pert_id** – list of pert_ids
- **pert_type** – list of pert_types. Avoid using only this parameter as the return could be very large.
- **cmap_name** – list of cmap_name, formerly pert_iname
- **cell_iname** – list of cell names
- **det_plates** – list of det_plates. det_plates values are the concatenation of values from

instinfo det_plate field with the 'l' delimiter used. :param build_name: list of builds :param return_fields: ['priority', 'all'] :param limit: Maximum number of rows to return :param table: table to query. This by default points to the level 5 siginfo table and normally should not be changed. :param verbose: Print query and table address. :return: Pandas Dataframe

cmapBQ.query.**get_bq_client**()

Return authenticated BigQuery client object.

Parameters **config** – optional path to config if not default

Returns BigQuery Client

cmapBQ.query.**get_table_info**(*client*, *table_id*)

Query a table address within client's permissions for schema.

Parameters

- **client** – Bigquery Client
- **table_id** – table address as {dataset}.{table_id}

Returns Pandas Dataframe of column names. Note: Not all column names are query-able but all will be returned from a given metadata table

cmapBQ.query.**list_cmap_compounds**(*client*)

List available compounds

Parameters **client** – BigQuery Client

Returns Single column Dataframe of compounds

cmapBQ.query.**list_cmap_moas**(*client*)

List available MoAs

Parameters **client** – BigQuery Client

Returns Single column Dataframe of MoAs

cmapBQ.query.**list_cmap_targets**(*client*)

List available targets

Parameters **client** – BigQuery Client

Returns Pandas DataFrame

cmapBQ.query.**list_tables**()
Print table addresses. Comes from defaults in config.

Returns None

cmapBQ.query.**run_query**(*client*, *query*)
Runs BigQuery queryjob

Parameters

- **client** – BigQuery client object
- **query** – Query to run as a string

Returns QueryJob object

2.1.3 cmapBQ.utils module

cmapBQ.utils.**csv_to_gctx**(*filepaths*, *outpath*, *use_gctx=True*)

Convert list of csv files to gctx. CSVs must have 'rid', 'cid' and 'value' columns No other columns or metadata is preserved.

Parameters

- **filepaths** – List of paths to CSVs
- **outpath** – output directory of file
- **use_gctx** – use GCTX HDF5 format. Default is True

Returns

cmapBQ.utils.**long_to_gctx**(*df*)

Converts long csv table to GCToo Object. Dataframe must have 'rid', 'cid' and 'value' columns No other columns or metadata is preserved.

Parameters **df** – Long form pandas DataFrame

Returns GCToo object

2.2 Using CMap's BQ Toolkit

Introduction The cmapBQ toolkit enables access to data hosted in Bigquery directly from a python session.

2.3 Instructions for installing cmapBQ

The cmapBQ package is available on Pypi and can be installed using the command: `pip install cmapBQ`

2.4 Where to place your JSON service file

The recommended location for service account credentials is within the `~/.cmapBQ` folder. The following command will populate that folder with a `config.txt` file that points to your credentials file.

```
import cmapBQ.query as cmap_query
import cmapBQ.config as cmap_config

cmap_config.setup_credentials(path_to_json)
```

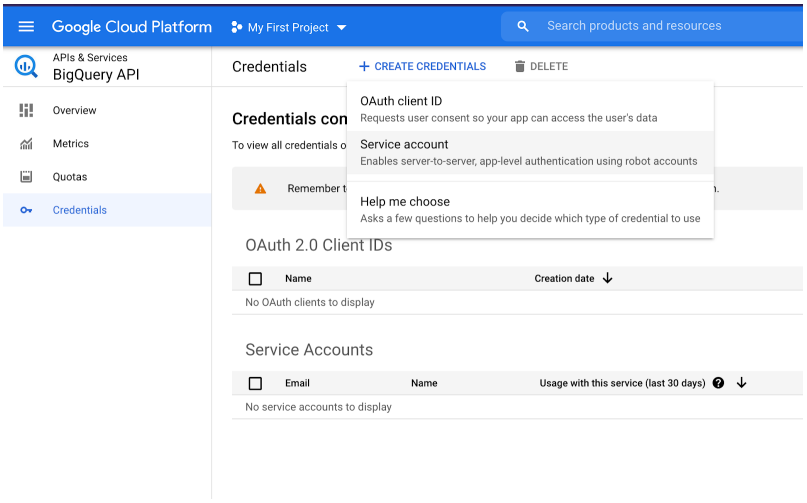
Tutorial Notebook available on Github

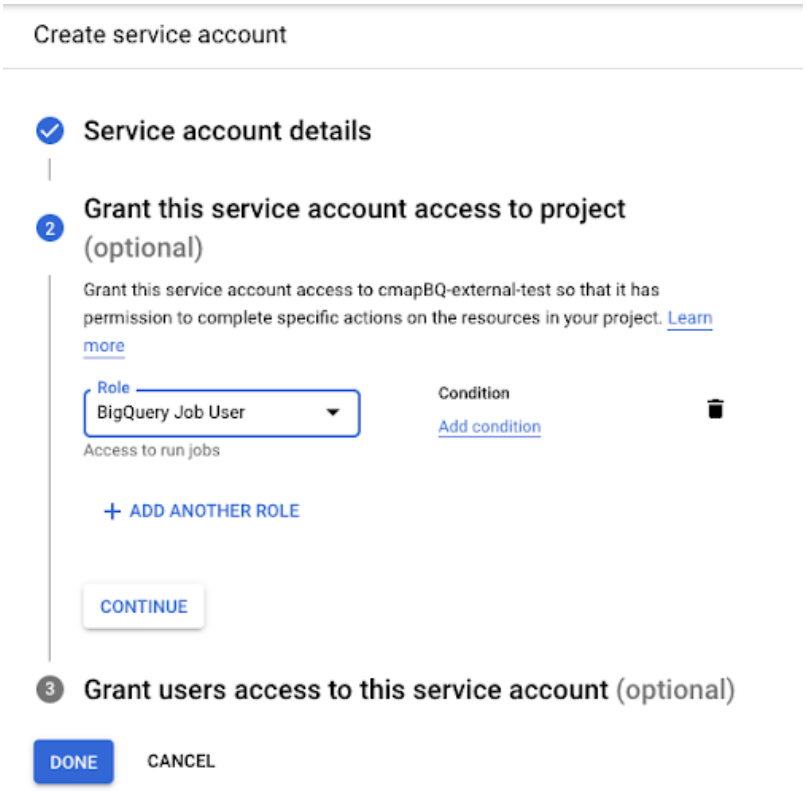
2.5 Credential's setup

To be able to access the dataset, register for a Google Cloud account. After registration or if you already have an account, go to your Google Cloud console and then activate your Google Cloud BigQuery API (link).

When you have access to your Google Cloud Account, go to APIs & Services > Credentials. Find the +Create Credentials and select "Service Account".

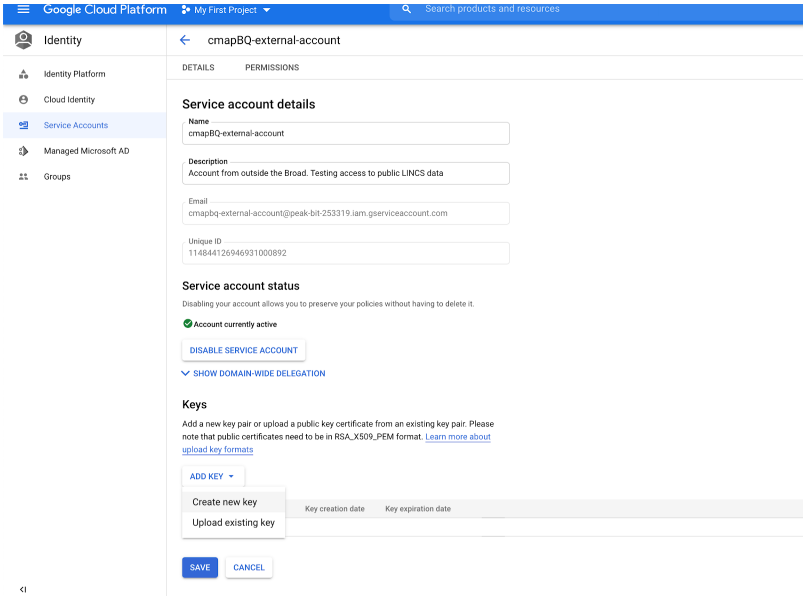
Note: Depending on your organization or project, you may not have access to the credentials page. If that is the case, discuss with the project admin to get your service account key, or create a new project in which you have permission.





Fill out service account details, make sure to set the Role to "BigQuery Job User"

After the service account has been created, find the Section labeled "Keys" and go to Add Key > Create new key. Select "JSON" format.



Place the downloaded JSON file in a safe location, for example, ~/.cmapBQ/ and run the following command in python once.

```
import cmapBQ.query as cmap_query
```

(continues on next page)

(continued from previous page)

```
import cmapBQ.config as cmap_config

cmap_config.setup_credentials(path_to_json)
```

Note: For usage in Colab, JSON key can be uploaded and referenced from the file viewer in the left side menu

2.6 Need Help?

For questions please add an issue to the External hyperlinks, like Github or email anup@broadinstitute.org

2.7 License

CHAPTER

THREE

INDICES AND TABLES

- genindex
- modindex

PYTHON MODULE INDEX

C

INDEX