Machine Learning Models Deployment using Sklearn2SQL framework

Technical Presentation

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https://github.com/antoinecarme/sklearn2sgl-demo



What is Sklearn2SQL?

- sklearn2sql is a "development tool" for generating deployment SQL code from scikit-learn objects.
 - https://github.com/antoinecarme/sklearn2sql-demo
- Using sklearn2sql, it is possible to predict values from an already-fitted classifier or a regressor simply by executing some SQL code.
- It can be seen as an alternative to PMML-based methods to perform In-database processing.
- It performs the deployment where the data are: in the database!!!
 - No data transfer is needed
 - An asset for performance and security.
 - SQL can also be validated and adapted before execution.
 - SQL is software: it can be integrated easily in large systems.
 - Easily distributable : one can generate SQL codes for all databases at the enterprise level and execute the same model with locally-adapted SQL codes.



Supported Machine Learning Models

- It is designed to support all classification and regression methods in scikit-learn
 - SVMs, linear models, naive-bayes. decision trees, MLP, etc
 - Transformers (PCA, imputers, scalers)
 - Feature selection
 - Outlier detection
 - Derived models (random forests, meta-estimators, pipelines, feature unions, ensembles, etc).



Supported Databases

- Support for most popular relational databases has been added progressively. Now, sklearn2sql supports almost all the leading relational databases referenced on DB-Engines.
 - https://db-engines.com/en/ranking/relational+dbms
- Open source databases : PostgreSQL (Just perfect !!!, most derived database), MariaDB (contributed some CTE-related bugs for this project. Very reactive team. All bugs were fixed !!!!
- Commercial databases : Oracle, MS SQL Server, IBM DB2, Teradata (to cover 95% of the market and get real-world tests)
- Embedded databases : SQLite (even in-memory ;). Nice for prototyping, documentation and development. Zero config. Available everywhere (on Android and iOS devices and inside jupyter notebooks ;).
- Hadoop databases : Hive and Impala
- Other: Firebird (low memory footprint. A stress test;), Monetdb (columnar, a SQL quality reminder;)



Sample Codes 1/4

- -- This SQL code was generated by sklearn2sql (development version).
- -- Copyright 2018
- -- Model : DecisionTreeClassifier
- -- Dataset : iris
- -- Database : mvsq
- -- This SQL code can contain one or more statements, to be executed in the order they appear in this file.
- -- Model deployment code

WITH 'DT_node_lookup' AS

`DT_node_data` AS

(SELECT 'Values'.node_id AS node_id, 'Values'.feature AS feature, 'Values'.threshold AS threshold, 'Values'.count, 'Values'.cogProba_1', 'Values'.parent_id, 'Values'.proba_0', 'Values'.proba_0', 'Values'.proba_0', 'Values'.proba_0', 'Values'.proba_1', 'Values'.proba_1', 'Values'.proba_1', 'Values'.proba_2', Values'.proba_2', Values'.p

FROM (SELECT 1.As node id. CAST(NULL AS CHAR(256)) As feature, NULL AS threshold, 37 AS count, 1.AS depth, 0.AS parent id. 1.0 AS 'Proba_0', 0.0 AS 'Proba_0', 0.0 AS 'Proba_0', 0.0 AS 'Proba_0', 1.0 AS 'Proba_0', 1.79769313486231e+308 AS 'LogProba_1', 0.0 AS 'Proba_0', 1.0 AS 'Proba_0', 1.79769313486231e+308 AS 'LogProba_0', 1.0 AS 'Proba_0', 1.0 AS 'Proba_0', 1.79769313486231e+308 AS 'LogProba_0', 0.0 AS 'Proba_0', 1.0 AS 'Proba_0', 1.79769313486231e+308 AS 'LogProba_0', 0.0 AS 'Proba_0', 1.79769313486231e+308 AS 'LogProba_0', 0.0 AS 'Proba_0', 0.0 AS 'Proba_0',

'DT_Output' AS

(SELECT 'DT_node_lookup'. 'KEY', 'AS 'KEY', 'DT_node_lookup'.node_id_2 AS node_id_2, 'DT_node_data'. 'proba_1', 'DT_node_data'. 'Proba_0' AS 'Node_0', 'DT_node_data'. 'LogProba_0', 'DT_node_data'. 'Proba_0', 'DT_node_data'. 'Proba_0', 'DT_node_data'. 'Proba_0', 'DT_node_data'. 'LogProba_2', 'DT_node_data'. 'LogProba_1', 'DT_node_data'. 'Proba_0', 'DT_node_data'. 'Proba_

FROM 'DT node lookup' LEFT OUTER JOIN 'DT node data' ON 'DT node lookup'.node id 2 = 'DT node data'.node id)

SELECT 'DT_Output'. 'KEY' AS 'KEY', NULL AS 'Score_0', NULL AS 'Score_2', 'DT_Output'. 'Proba_0' AS 'Proba_0', 'DT_Output'. 'Proba_1' AS 'Proba_1', 'DT_Output'. 'Proba_2' AS 'Proba_2', 'DT_Output'. 'LogProba_0' AS 'LogProba_0' AS 'LogProba_1' AS 'LogProba_1' AS 'LogProba_1', 'DT_Output'. 'Decision' AS 'Decision', 'DT_Output'. 'Decision' AS 'Decision', 'DT_Output'. 'Decision' AS 'Decision', 'DT_Output'. 'Proba_1' AS 'LogProba_2' AS 'LogProba_2', 'DT_Output'. 'Decision' AS 'LogProba_1' AS 'L

FROM `DT_Output



Sample Codes 2/4

https://github.com/antoinecarme/sklearn2sql-demo/blob/master/VeryLargeModelsSupport_temp_tables/XGBClassifier/FourClass_500/pgsql/demo3_XGBClassifier_pgsql.sql

```
-- This SOL code was generated by sklearn2sgl (development version).
              -- Copyright 2018
              -- Model : XGBClassifier
              -- Dataset : FourClass 500
             -- Database : pgsgl
              -- This SOL code can contain one or more statements, to be executed in the order they appear in this file.
           -- Code For temporary table TMP 20180417010516 0ECOBE XGB B0 part 1/2. Create
15
           CREATE TEMPORARY TABLE "TMP 20180417010516 0ECOBE XGB B0" (
                               "KEY" BIGINT.
17
18
                              "Score_0" FLOAT,
                              "Score 1" FLOAT,
                              "Score 2" FLOAT,
21
                              "Score 3" FLOAT
22
23
             ON COMMIT PRESERVE ROWS
                           ary_max_ctc A3
                           (SELECT score soft max."KEY" AS "KEY", score soft max."Score 0" AS "Score 0", score soft max."Score 1", score soft max."Score 2" AS "Score 2", score
                           FROM score soft max LEFT OUTER JOIN (SELECT union with max. "KEY" AS "KEY Score", min(union with max.class) AS "arg max Score"
           1060
           1061
                           FROM union with max
                           WHERE union_with_max."Score" >= union_with_max."max_Score" GROUP BY union_with_max."KEY") AS "arg_max_t_Score" ON score_soft_max."KEY" = "arg_max_t_Score"."KEY
           1062
                           FROM score soft max) AS soft max comp ON soft max comp."KEY softmax" = "arg max t Score"."KEY Score")
           1063
                             SELECT arg max cte. "KEY" AS "KEY", CAST(NULL AS FLOAT) AS "Score 0", CAST(NULL AS FLOAT) AS "Score 1", CAST(NULL AS FLOAT) AS "Score 2", CAST(NULL AS FLOAT) AS "Score 1", CAST(NULL AS FLOAT) AS "Score 2", CAST(NULL AS FLOAT) AS "Score 1", CAST(NULL AS FLOAT) AS "Score 2", CAST(NULL AS FLOAT) AS "Score 2", CAST(NULL AS FLOAT) AS "Score 1", CAST(NULL AS FLOAT) AS "Score 2", CAST
           1064
           1065
                           FROM arg_max_cte
```

Sample Codes 3/4 1 -- This SQL code was generated by sklearn2sql (development version)

```
2 -- Copyright 2018
4 -- Model : GaussianNB_Pipeline
5 -- Dataset : BinaryClass_10
  -- Database : oracle
9 -- This SOL code can contain one or more statements, to be executed in the order they appear in this file.
```

```
13 -- Code For temporary table 22737 HHC6Q9 ADS IMP 1 OUT part 1/2. Create
15
16 CREATE GLOBAL TEMPORARY TABLE "22737 HHC609 ADS IMP 1 OUT" (
           "KEY" NUMBER (19) NOT NULL
          impter 2 BINARY DOUBLE.
          impter 3 BINARY DOUBLE
          impter 4 BINARY DOUBLE.
           impter 9 BINARY DOUBLE.
           impter 10 BINARY DOUBLE.
           impter 11 BINARY DOUBLE.
           PRIMARY KEY ("KEY")
29 )
```

```
-- Code For temporary table 22737_HHC6Q9_ADS_IMP_1_OUT part 2/2. Populate
```

```
34
                                       INSERT INTO "22737_HHC6Q9_ADS_IMP_1_OUT" ("KEY", impter_2, impter_3, impter_5, impter_6, impter_7, impter_8, impter_9, impter_10, impter_11) SELECT "U
                                       FROM (SELECT "ADS_imp_1_OUT"."KEY", "ADS_imp_1_OUT".impter_2, "ADS_imp_1_OUT".impter_3, "ADS_imp_1_OUT".impter_4, "ADS_imp_1_OUT".impter_5, "ADS_imp
                                      FROM (SELECT "ADS". "KEY" AS "KEY", CASE WHEN ("ADS". "Feature_0" IS NULL) THEN 0.061829205238134496 ELSE "ADS". "Feature_0" END AS impter_2, CASE WHEN ("ADS". "Feature_0" IS NULL) THEN 0.061829205238134496 ELSE "ADS". "Feature_0" END AS impter_2, CASE WHEN ("ADS". "Feature_0" IS NULL) THEN 0.061829205238134496 ELSE "ADS". "Feature_0" END AS impter_2, CASE WHEN ("ADS". "Feature_0" IS NULL) THEN 0.061829205238134496 ELSE "ADS". "Feature_0" END AS impter_2, CASE WHEN ("ADS". "Feature_0" IS NULL) THEN 0.061829205238134496 ELSE "ADS". "Feature_0" END AS impter_2, CASE WHEN ("ADS". "Feature_0" IS NULL) THEN 0.061829205238134496 ELSE "ADS". "Feature_0" END AS impter_2, CASE WHEN ("ADS". "Feature_0" END AS impter_2, CASE WHEN (
                                      FROM "BINARYCLASS 10" "ADS") "ADS imp 1 OUT") "U"
```

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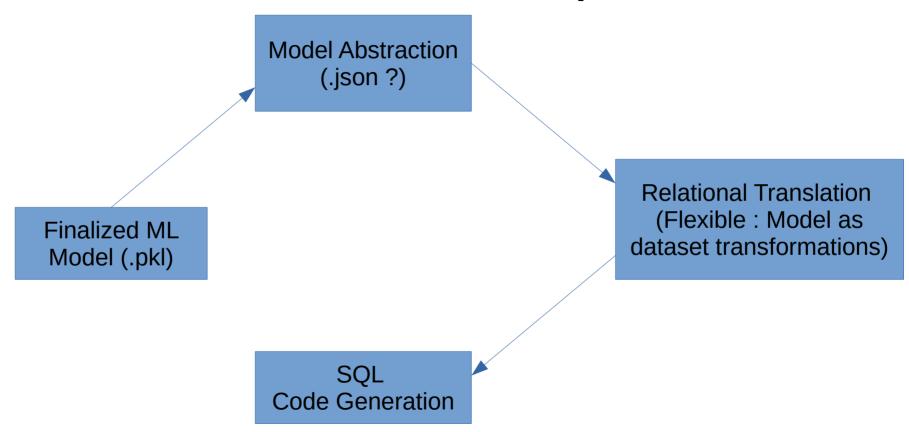
```
99 arg max cte AS
              (SELECT score_soft_max."KEY" AS "KEY", score_soft_max."Score_0" AS "Score_0", score_soft_max."Score_1", score_soft_max."Proba_0" AS "Proba_0", score_soft_max."Score_1", score_soft_max."Proba_0" AS "Proba_0", score_soft_max."Score_1", score_soft_max."Proba_0" AS "Proba_0", score_soft_max."Score_1", score_soft_max."Proba_0", score_soft_max."Score_1", score_soft_max."Proba_0", score_soft_max."Score_1", score_soft_max."Proba_0", score_soft_max."Score_1", score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Score_soft_max."Sco
101 FROM score_soft_max LEFT OUTER JOIN (SELECT union_with_max."KEY" AS "KEY_Score", min(union_with_max.class) AS "arg_max_Score"
102 FROM union with max
               WHERE union with max. "max Score" <= union with max. "Score" GROUP BY union with max. "KEY") "arg max t Score" ON score soft max. "KEY" = "arg max t Score". "KEY Sco
                   FROM score_soft_max) soft_max_comp ON soft_max_comp."KEY_softmax" = "arg_max_t_Score"."KEY_Score")
                      SELECT arg_max_cte."KEY" AS "KEY", CAST(NULL AS BINARY_DOUBLE) AS "Score_0", CAST(NULL AS BINARY_DOUBLE) AS "Score_1", arg_max_cte."SoftProba_0" AS "Proba_0",
                   FROM arg_max_cte
```



Sample Codes 4/4

```
1 -- This SQL code was generated by sklearn2sql (development version).
    -- Copyright 2018
    -- Model : SVR rbf
   -- Dataset : boston
   -- Database : sqlite
    -- This SQL code can contain one or more statements, to be executed in the order they appear in this file.
10
11
12
    -- Model deployment code
14
    WITH kernel input AS
    (SELECT "ADS". "KEY" AS "KEY", CAST("ADS". "Feature_0" AS FLOAT) AS "Feature_1" AS FLOAT) AS "Feature_1", CAST("ADS". "Feature_2" AS FLOAT)
    FROM boston AS "ADS").
    "SV data" AS
    (SELECT "Values".sv idx AS sv idx, CAST("Values".dual coeff AS FLOAT) AS dual coeff, CAST("Values".sv 0 AS FLOAT) AS sv 0, CAST("Values".sv 1 AS FLOAT) AS sv 1,
    FROM (SELECT 0 AS sv_idx, 0.1 AS dual_coeff, 0.11425 AS sv_0, 0.0 AS sv_1, 13.89 AS sv_2, 1.0 AS sv_3, 0.55 AS sv_4, 6.373 AS sv_5, 92.4 AS sv_6, 3.3633 AS sv_7
    kernel dp AS
    (SELECT t. "KEY" AS "KEY", t.dot product AS dot product
    FROM (SELECT full join data sv. "KEY" AS "KEY", sum(CAST(full join data sv.dot prod1 AS FLOAT)) + 21.35026686098341 AS dot product
    FROM (SELECT kernel_input."KEY" AS "KEY", "SV_data".dual_coeff * exp(min(max(-100.0, -0.07692307692307693 * (power(kernel_input."Feature_0" - "SV_data".sv_0, 2)
    FROM kernel_input, "SV_data") AS full_join_data_sv GROUP BY full_join_data_sv."KEY") AS t)
     SELECT kernel dp. "KEY" AS "KEY", kernel dp.dot product AS "Estimator"
    FROM kernel dp
```

Framework Description





System Input

- The system generates SQL code from already trained models.
- The gory details of the training process are not significant.
- Almost all public interfaces and web services take a serialized model as input (pickle is your friend here).



Model Abstraction

- In this step, the system performs a complete formal abstraction of the underlying algorithm of the model.
 - For a linear Model:
 - {"Type": "linear", "coefficients": [8.88, 8888e-8], "intercept": 888888}
- More complex formal abstractions are available for each model/algorithm type (DT, XGB, SVM, RF, Pipeline, ...).
- The abstraction must be complete, For a random forest (RF) model, the abstraction contains the individual abstractions of all the forest decision trees.
- Adding a new mathematical model requires designing/authoring these abstractions.
 - The math behind scikit-learn algorithms (and machine learning in general) is evolving slowly (need many years to "invent" a new model). Almost all of these models date back to 19xx.
 - Scikit-learn has a lot of requirements on what model can be added (popularity, publications, citations, impact,), and that's really good. https://scikit-learn.org/stable/fag.html
 - The current version of the sklearn2sql framework has designed (> 40) abstractions of almost all scikit-learn models known before 2020.
 - https://scikit-learn.org/stable/modules/classes.html
- These abstractions are deduced from a reloaded/living model. We only use model metadata. The original dataset is not needed even if the model can help generating/simulating one.
- The formal abstraction is expressed in JSON format.
 - Almost all python objects have a dict member. Python object introspection is easy.
 - Scikit Learn Models are aggregates of numpy python objects.
 - XGB models already have a to_json method. Easy.
 - JSON code is debuggable.



Relational Model Representation

- All machine learning data processing can be performed using sequences of simple dataset/columns transformations (dataset → dataset mapping).
- This translation is performed only using the "Complete" Model Abstraction (JSON format is enough).
- These dataset transformations can be translated into relations (as in a relational algebra / SQL).
- For a given model, The number of these transformations depends on the complexity of the model.
 - Think of these as the layers of a sequential neural network (Scikit MLP), but at a lower level.
- Individual transformations are developed using specialized python classes, with the most tasks done at the abstract level.
 - The transformation does not take into account the type of model it is part of.
 - Groups of transformations used to compute the predicted values (arg-max of probabilities) are shared across all model representations (the same SQL code between DTs and pipelines of SVMs).
- A scikit-learn machine learning model can be mapped this way.
 - A decision tree score computation can be performed by hand using ~4 excel sheets, and these sheets can be mapped to SQL tables/views. The first table contains the input and the last contains the scores and class probabilities as columns.
 - A random forest with 500 trees, will be translated as ~4*500 separate relations. An additional relation is used to compute the RF class probabilities (means of 500 individual class probabilities).
 - · Seems too mechanical. There are some technical limitations but SQL allows the usage of views or temporary tables to deal with this kind of complexity.



SQL Code Generation 1/4

- SQL Code generation is about translation the model representation into a valid SQL code for a target database dialect.
- We use the excellent Python SQLAlchemy as a framework for handling relational model representions internal transformations.
 - https://www.sqlalchemy.org/
- SQLAlchemy allows mapping each transformation to a set of SQLAlchemy objects (table, expression, column, function, join, literal values, case, union, ...)
- SQLAlchemy Expressions can generate their SQL Code for a target database which has a python SQLAlchemy driver.
- SQLAlchemy has a set of internally supported database drivers (psql, sqlite, mssql, oracle, ...)
- Almost all database vendors maintain a python SQLAlchemy driver for their database (teradata, ...).
 - Easy to add a new database.
 - For teradata : https://github.com/Teradata/sqlalchemy-teradata
- SQLAlchemy plays nicely with pandas
 - One can create a pandas dataframe using a SQLAlchemy connection and a SQL select statement to be executed.
 - https://pandas.pydata.org/docs/reference/api/pandas.read_sql.html#pandas.read_sql
 - One can save a dataframe as a table through a SQLAlchemy database connection.
 - $\bullet \ https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.to_sql.html\#pandas.DataFrame.to_sql.html\#pandas.DataFrame.to_sql.html#pandas.DataFrame.to_sql$



SQL Code Generation 2/4

Sketch of a linear regression model SQL code generation

```
import sqlalchemy as sa
input_cte = sa.Table("boston")
scal_prod_expr = input_cte.columns["Feature1"] * sa.literal_value(coefs[1]) + ...
scal_prod_expr = scal_prod_expr + input_cte.columns["Feature4"] * sa.literal_value(coefs[4])
scal_prod_expr = scal_prod_expr + sa.literal_value(intercept)
estimator = sa.cast_as_float(scal_prod_expr)
output_cte = sa.cte([ input_cte.columns["KEY"] , estimator.label("Estimator") ])
select_est = sa.select(output_cte)
# All the code above is database-agnostic,
lSQL = select_est.generate_sql(psql_connection)
```



SQL Code Generation 3/4

- By default, each transformation is generated as a CTE through an sa.CTE object (WITH clause)
 - https://modern-sql.com/feature/with
- For a simple model, a single select statement which contains one or many CTEs is generated.
 - SQL Code = [With Clauses + compute_scores_select]
- Some databases do not support too many WITH clauses in the same select
 - MariaDB, number of CTEs > 64.
 - https://jira.mariadb.org/browse/MDEV-13730
- For complex models (number of CTEs > 64), the SQL generator materializes some CTEs
 - For a RF model with 500 trees, each tree is generated as temporary table instead of a CTE. These temporary tables are populated on each code execution and automatically dropped by internal database mechanisms.
 - SQL Codes = [500*create temp tables, 500*populate temp tables, 1*aggregate scores select]



SQL Code Generation 4/4

- For the SQL code design, the author tried when possible to use meaningful aliases in the SQL code. The names are intention revealing according to the excellent Modern SQL.
 - http://modern-sql.com/use-case/literate-sql
- For example, a SQL generated from a decision tree contains three common table expressions (CTEs) whose names are: "DT_node_lookup", "DT_node_data" and "DT_Output.
 - https://github.com/antoinecarme/sklearn2sql-demo/blob/master/sample_outputs_tuning_round_1/DecisionTreeClassifier/iris/pgsql/demo2_DecisionTreeClassifier_pgsql.sql
- This design has a significant impact on the performance. All SQL codes are tested to execute in less than 2-3 minutes on the various databases, even for very complex models.



Quality Assessment 1/2

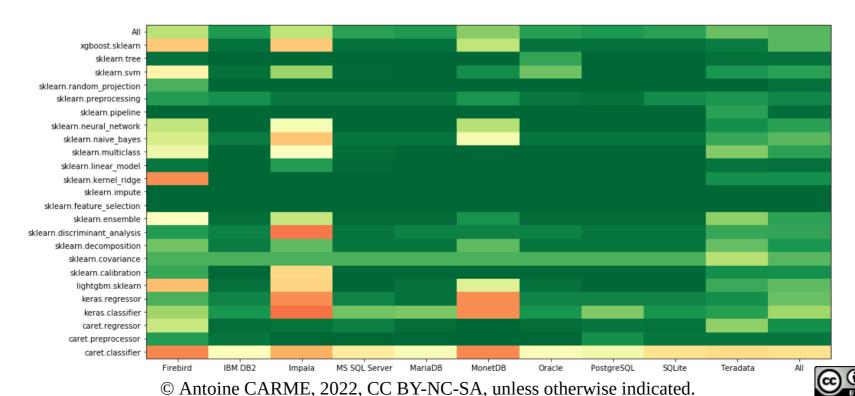
- A test framework has been put in place.
- The framework works on all supported databases instances simultaneously.
- For each scikit-learn model class, we perform the following tests:
 - Train different models on datasets of various sizes (nrows, ncols). These datasets are transferred
 - For each trained model :
 - save it,
 - Predict all the possible values for all the training dataset in python scikit-learn (sklearn_output_python_df)
 - generate the SQL,
 - Execute the SQL code on each database => pandas dataframes (gen_sql_output_mssql_df , ...).
 - Compare the relevant output columns between sklearn_output_python_df and each database output dataframe.
 - Add some reporting for success/failures each model/database combination.



Quality Assessment 2/2

• Sample report :

https://github.com/antoinecarme/sklearn2sql_heroku/blob/master/Quality/extensive_tests-debrief.ipynb



Extensions

- The system has been designed to been extended to support additional types of models:
 - Gradient Boosting Models: XGBoost and LightGBM
 - · Have a scikit-learn API.
 - These can be exported in a json format.
 - Keras and PyTorch Deep Learning Models
 - Both share the same abstraction layers.
 - https://github.com/antoinecarme/keras2sql
 - https://github.com/antoinecarme/pytorch2sql
 - Defined new transformations for NN Layers and transfer functions (ReLU, ...).
 - · Basically he same as sklearn.MLP
 - Support Convolutional networks (partial) and recursive models (RNN, LSTM, GRU)
 - R Models, through Caret.
 - Basically, these are the same as the existing scikit-learn models
 - https://github.com/antoinecarme/caret2sql
 - We chose to generate code for "equivalent" abstractions for scikit-learn models.
 - Abstract models are generated by running custom R model introspection scripts.
 - The four NN dense layer implementations (sklearn.MLP, Keras.Dense, PyTorch.Dense, Caret.nnet) share the same abstraction and the model transformations.
 - These models have been included in the Quality Assessment test framework.
 - R models output (using R) is compared with the generated SQL output for each database.



谢谢!!!!

