Data Science with PostgreSQL

Balázs Bárány

Data Scientist

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Contents

Sexiest job of the 21st century

- According to Google, LinkedIn, ...

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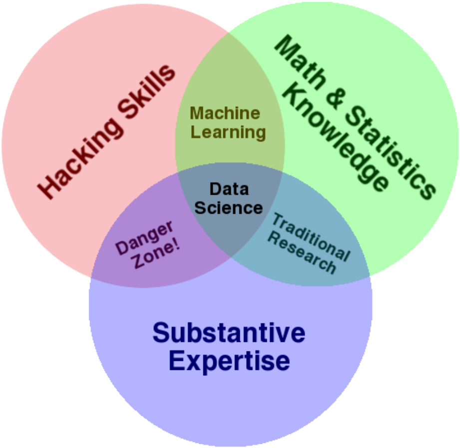
- According to Google, LinkedIn, ...
- Who is a Data Scientist?

Data Science Venn Diagram



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Tasks of data scientists

- Get data from various sources
  - Big data?

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- Analyze & visualize
- Predict & prescribe
- Operationalize

The Data Mining process

Cross Industry Standard Process for Data Mining (Kenneth Jensen/Wikimedia Commons)

Tools and methods

Tools and methods

Scripting and programming

- R
- Python with extensions
- Octave/Matlab, other mathematic languages
- Hadoop and Big Data programming libraries (mostly Java)
- Cloud services

Integrated GUI tools

- (partly) Open Source: RapidMiner, KNIME, Orange
- Data Warehouse tools extended for analytics: Pentaho, Talend
- Many commercial tools, e. g. SAS, IBM SPSS
- Hadoop-related newcomers: e. g. Datameer

Data Infrastructure

- Databases and data stores
  - Relational, NoSQL
  - Hadoop clusters
  - In-memory
- Data streams
- Free-form data: text, images, video, audio, ...
- Web APIs
- Open Data

Data acquisition and preprocessing

- Data ingestion in raw format

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  - Missing values
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  - Missing values
  - Abnormal values
- Result: data set suitable for analytics

Predictive Modeling

- Supervised and unsupervised methods
  - Target variable known or not

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Predictive Modeling

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  - Target variable known or not
- Classification (supervised): Prediction of a class or category
- Regression (supervised): Prediction of numeric value
- Clustering (unsupervised): Automatic "grouping" of data
- Association analysis, outlier detection, time series prediction, ...

Deployment and operationalization

- Model application to new data => prediction + confidence
- What to do with predictions?

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- Store in ERP or CRM
- Tell someone (email, popup)
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- Interrupt financial transaction => prescription
- Order supplies => prescription
- ...

Data Science with PostgreSQL

Doing Data Science with PostgreSQL

Caveats

- This stuff is not easy

Caveats

- This stuff is not easy
- Must be root and postgres
  - Maintain your PostgreSQL yourself
  - Able to compile stuff

Caveats

- This stuff is not easy
- Must be root and postgres
  - Maintain your PostgreSQL yourself
  - Able to compile stuff
- You should ask ;-)
  - your boss
  - co-workers
  - customer

Data Science with PostgreSQL

Business & data understanding

Business understanding

- What is the purpose of the business?
- What are existing processes?
- Drivers of business success

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- Project goals and challenges
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- Not a technical activity, PostgreSQL can't help much

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- Existing data
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  - Complete? Correct? In suitable form?
  - Usable? (regulations, access constraints, ...)

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  - Simple or complex IDs
- Data size
  - Too small
  - Too big
- Suitability for predictive modeling
  - Target variable?
  - Attribute types

Data understanding with PostgreSQL

- Get data into PostgreSQL
  - Classical import process
  - Foreign Data Wrappers

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- Analyze data distribution
  - Group by and aggregate
    - Count, Count Distinct, Min, Max
  - Count NULLs
  - Search for missing links (incomplete foreign keys)

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- Analyze data distribution
  - Group by and aggregate
    - Count, Count Distinct, Min, Max
  - Count NULLs
  - Search for missing links (incomplete foreign keys)
- Analyze "surprizes"
  - Impossible values
  - Missing values in "required" fields

Data understanding with PostgreSQL – summary

- Good SQL knowledge required
- Tedious manual process
  - repetitive
  - not suitable for large number of attributes
- No built-in visualization

Data understanding with PostgreSQL – summary

- Good SQL knowledge required
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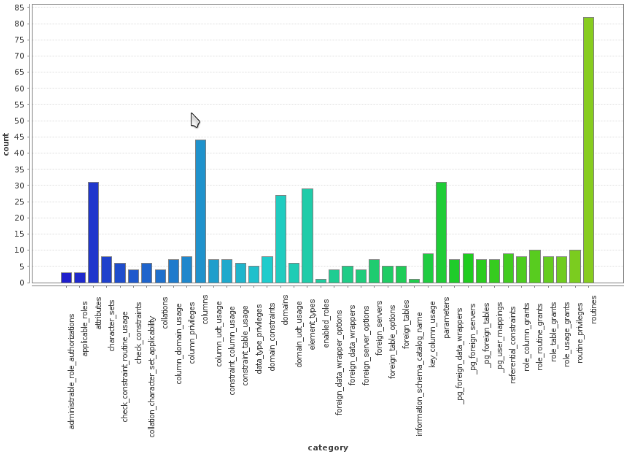
- Or maybe...

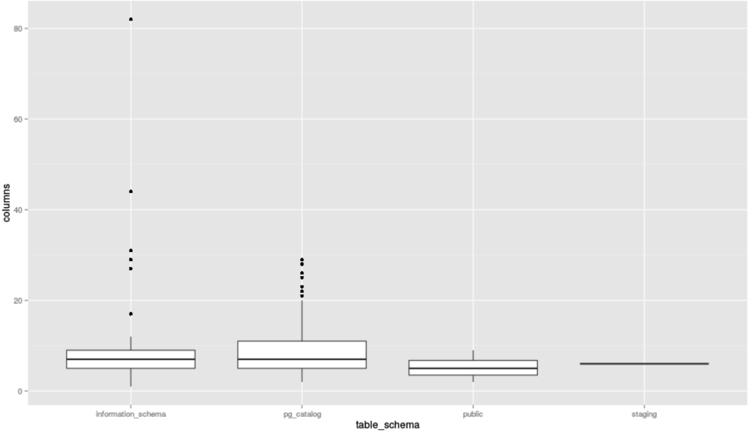
SQL barchart output

```
foreign_table_options              |   5 | ###
foreign_tables                     |   5 | ###
information_schema_catalog_name    |   1 |
key_column_usage                   |   9 | #####
parameters                         |  32 | ###################
_pg_foreign_data_wrappers          |   7 | ####
_pg_foreign_servers                |   9 | #####
_pg_foreign_table_columns          |   4 | ##
_pg_foreign_tables                 |   7 | ####
_pg_user_mappings                  |   7 | ####
referential_constraints            |   9 | #####
role_column_grants                 |   8 | ####
role_routine_grants                |  10 | ######
role_table_grants                  |   8 | ####
role_udt_grants                    |   7 | ####
role_usage_grants                  |   8 | ####
routine_privileges                 |  10 | ######
routines                           |  82 | ##################################################
schemata                           |   7 | ####
sequences                          |  12 | #######
sql_features                       |   7 | ####
sql_implementation_info            |   5 | ###
sql_languages                      |   7 | ####
sql_packages                       |   5 | ###
sql_parts                          |   5 | ###
sql_sizing                         |   4 | ##
sql_sizing_profiles                |   5 | ###
```

Bar chart from GUI tool



Boxplot output



Data understanding wrap up

- DBMS not built for this
- It can support more specialized tools

Data understanding wrap up

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- Introduction: R
  - "A free software environment for statistical computing and graphics"
  - Available in PostgreSQL

PL/R: A statistical language for PostgreSQL

- R as a standalone language
  - Mathematical and statistical methods
  - Powerful visualization functions
  - Classical, modern and bleeding edge modeling
  - Arrays and data frames are central data types
  - Operates only in memory

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  - Classical, modern and bleeding edge modeling
  - Arrays and data frames are central data types
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- PL/R: R as a loadable procedural language for PostgreSQL
  - First released in 2003 by Joe Conway
  - License: GPL

R usage outside of PostgreSQL

- Development environments
  - RStudio (AGPL or commercial, local & web)
  - RKWard, Cantor (KDE projects)
  - StatET (Eclipse)
- Frontends
  - R Commander
  - Deducer
  - Rattle
- Web framework: Shiny (AGPL or commercial)

Working with R in PostgreSQL

- Install functions in the database

Example

```
select install_rcmd('
    myfunction <-function(x)
      {print(x)}
');
```

- Install without function body

Example

```
CREATE FUNCTION rnorm
  (n integer, mean double precision, sd double precision)
RETURNS double precision[]
AS ''
LANGUAGE 'plr';
```

Using R in PostgreSQL for data understanding

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- Data distributions
- Advanced statistics

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- Execution outside
  - Simple and interactive, but data transfer

Data Science with PostgreSQL

Preprocessing

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- What databases are built for

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- Rows: very dynamic
  - Easy to create new rows by joining
  - Easy to filter
- Columns: not so much
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- Rows: very dynamic
  - Easy to create new rows by joining
  - Easy to filter
- Columns: not so much
  - Easy to create new columns
  - Only explicit access
- Wider interpretation of preprocessing
  - Enrichment with external data
  - New attributes from existing ones
  - Recoding, recalculation
  - Missing value handling

Preprocessing: organizing workflow

- Common Table Expressions
  - organize processing steps
  - partial and intermediate results

Example

```
WITH source AS (
  SELECT *, ROW_NUMBER() OVER () AS rownum
  FROM source_table
),
no_missings AS (
  SELECT *
  FROM source
  WHERE field1 IS NOT NULL
    AND field2 IS NOT NULL
)
etc.
```

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- Much easier in SQL than programming languages and data mining tools

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  - NoSQL databases (MongoDB, Cassandra, CouchDB, Redis, ...)

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  - Files (CSV, ZIP, JSON, ...)

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  - Network sources - Multicorn (RSS, IMAP, Twitter, S3, ...)
  - Files (CSV, ZIP, JSON, ...)
  - Write your own in C or Python or Ruby

Data Science with PostgreSQL

Modeling

Model development

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  - Naive Bayes, Linear Regression
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- Some attempts to build them
  - Naive Bayes, Linear Regression
  - Difficult for more advanced algorithms
- Better done in specialized language or tool
  - PL/R
  - PL/Python

PL/Python

- Python procedural language available in PostgreSQL
- scikit-learn: Machine learning toolbox for Python
  - Classification, regression, clustering
  - Model selection, validation
  - Preprocessing
- matplotlib: Generic and statistical plotting library

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- Python procedural language available in PostgreSQL
- scikit-learn: Machine learning toolbox for Python
  - Classification, regression, clustering
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  - Preprocessing
- matplotlib: Generic and statistical plotting library
- PL/Python is an alternative to PL/R

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Evaluation of modeling results

- Models return predictions
- Prediction can be compared to known result (target variable)
- Measures of model performance: Accuracy, precision, recall, ...

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- Split validation
- Cross validation

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  - do more preprocessing
  - select better classifier
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- Cycle: preprocessing - modeling - evaluation
- Better done in data mining environment

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  - Less overhead

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  - Instant application using triggers
  - Well-known execution environment
  - Functionality available over standard interface
- Some models easily expressed in SQL

Deployment of PL/R or PL/Python models

- Model developed in database or outside

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- Put into global context
  - PL/R: load("saved object", .GlobalEnv)
  - PL/Python: Global dictionary "GD"
- Application function in matching language
  - Uses existing model
  - Returns target variable

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  - Returns target variable
- Trigger func or UPDATE uses application function

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Summary

- PostgreSQL's support for data science tasks
  - Best: preprocessing, deployment
- Modern SQL for preprocessing
- Foreign Data Wrappers for data integration
- Procedural languages for data mining

Questions?

- Balázs Bárány, <balazs@tud.at>
- https://datascientist.at/