Data Science with PostgreSQL

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Data Scientist

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  Business & data understanding
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  Deployment

Summary
Sexiest job of the 21st century

- According to Google, LinkedIn, ...
Sexiest job of the 21st century

- According to Google, LinkedIn, ...

- Who is a Data Scientist?
Data Science Venn Diagram

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Introduction — What is Data Science?

Tasks of data scientists

- Get data from various sources
  - Big data?
Tasks of data scientists

- Get data from various sources
  - Big data?
- Mash up & format for analysis
Introduction – What is Data Science?

Tasks of data scientists

- Get data from various sources
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- Mash up & format for analysis
- Analyze & visualize
Tasks of data scientists

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- Analyze & visualize
- Predict & prescribe
Tasks of data scientists

- Get data from various sources
  - Big data?
- Mash up & format for analysis
- Analyze & visualize
- Predict & prescribe
- Operationalize
The Data Mining process

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

Tools and methods of Data Scientists

Data acquisition and preprocessing

- Data ingestion in raw format

- Joining, aggregating, filtering, calculating, ...
Data acquisition and preprocessing

- Data ingestion in raw format
- Joining, aggregating, filtering, calculating, ...
Data acquisition and preprocessing

- Data ingestion in raw format
- Joining, aggregating, filtering, calculating, ...
- Data cleansing
  - Missing values
  - Abnormal values
Data acquisition and preprocessing

- Data ingestion in raw format
- Joining, aggregating, filtering, calculating, ...
- Data cleansing
  - Missing values
  - Abnormal values
- Result: data set suitable for analytics
Predictive Modeling

- Supervised and unsupervised methods
  - Target variable known or not
Predictive Modeling

- Supervised and unsupervised methods
  - Target variable known or not
- Classification (supervised): Prediction of a class or category
- Regression (supervised): Prediction of numeric value
Predictive Modeling

- Supervised and unsupervised methods
  - 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?
Deployment and operationalization

- Model application to new data => prediction + confidence
- What to do with predictions?
  - Store in ERP or CRM
  - Tell someone (email, popup)
  - Add a label (e.g. mark email as spam)
Deployment and operationalization

- Model application to new data $\Rightarrow$ prediction + confidence
- What to do with predictions?
- Store in ERP or CRM
- Tell someone (email, popup)
- Add a label (e.g. mark email as spam)
- Interrupt financial transaction $\Rightarrow$ prescription
- Order supplies $\Rightarrow$ prescription
- ...
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
Business understanding

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

Not a technical activity, PostgreSQL can't help much
Business understanding

- What is the purpose of the business?
- What are existing processes?
- Drivers of business success
- Project goals and challenges
- Availability of data and resources
- Success criteria
Business understanding

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Data understanding

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

Connecting separate data sources
- Simple or complex IDs
- Data size
  - Too small
  - Too big

Suitability for predictive modeling
- Target variable?
- Attribute types
Data understanding

- **Existing data**
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- **Connecting separate data sources**
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Data understanding with PostgreSQL

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

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

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

- Get data into PostgreSQL
  - Classical import process
  - Foreign Data Wrappers
- Analyze data distribution
  - Group by and aggregate
    - Count, Count Distinct, Min, Max
  - Count NULLs
  - Search for missing links (incomplete foreign keys)
- Analyze “surprises”
  - 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
- Tedious manual process
  - repetitive
  - not suitable for large number of attributes
- No built-in visualization
- Or maybe...
### SQL bar chart output

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<th>Foreign Tables</th>
<th>Information Schema Catalog Name</th>
<th>Foreign Table Options</th>
<th>Key Column Usage</th>
<th>Parameters</th>
<th>Pg Foreign Data Wrappers</th>
<th>Pg Foreign Servers</th>
<th>Pg Foreign Table Columns</th>
<th>Pg Foreign Tables</th>
<th>Pg User Mappings</th>
<th>Referential Constraints</th>
<th>Role Column Grants</th>
<th>Role Routine Grants</th>
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<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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

- DBMS not built for this
- It can support more specialized tools
- 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
PL/R: A statistical language for PostgreSQL

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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

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

- Install without function body

Example

```sql
CREATE FUNCTION rnorm
    (n integer, mean double precision, sd double precision)
RETURNS double precision[]
AS ''
LANGUAGE 'plr';
```
Using R in PostgreSQL for data understanding

- Advanced visualization
- Data distributions
- Advanced statistics
Using R in PostgreSQL for data understanding

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- Data distributions
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- Execution in the database
  - Clumsy, but direct data access
Using R in PostgreSQL for data understanding

- Advanced visualization
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- Advanced statistics
- Execution in the database
  - Clumsy, but direct data access
- Execution outside
  - Simple and interactive, but data transfer
Preprocessing

- What databases are built for
Preprocessing

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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
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- 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

```sql
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.
```
Preprocessing: attribute creation

- Aggregation

  ▶ Partial aggregation by window functions
  ▶ In-group measures, e.g. ratio \( \frac{att}{\text{SUM}(att)} \) OVER (PARTITION BY ...)
  ▶ In-group numbering \( \text{ROW_NUMBER()} \) OVER (PARTITION BY ... ORDER BY ...)
  ▶ Comparing to previous/next value \( att - \text{LAG}(att, 1) \) OVER (ORDER BY ...)

  Much easier in SQL than programming languages and data mining tools
Preprocessing: attribute creation

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  - In-group measures, e.g. ratio
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Preprocessing: enrichment

- PostGIS for geodata
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- Foreign data wrappers (see PostgreSQL Wiki)
Preprocessing: enrichment

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  - Other databases (other PostgreSQL server, MySQL, Oracle, MSSQL, JDBC, SQL Alchemy ...)
  - NoSQL databases (MongoDB, Cassandra, CouchDB, Redis, ...)

Data Science with PostgreSQL

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- Write your own in C or Python or Ruby
Data Science with PostgreSQL

Model development

- Machine learning algorithms not well suited for SQL
Model development

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- Some attempts to build them
  - Naive Bayes, Linear Regression
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- 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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- matplotlib: Generic and statistical plotting library
- PL/Python is an alternative to PL/R
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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- If not good enough,
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- Cycle: preprocessing - modeling - evaluation
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- Some models easily expressed in SQL
Deployment of PL/R or PL/Python models

- Model developed in database or outside
Deployment of PL/R or PL/Python models

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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

Trigger function or `UPDATE` uses the application function.
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Summary

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

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