EARL US Roadshow | November, 2018

R-bots for Data Science Workflow Automation

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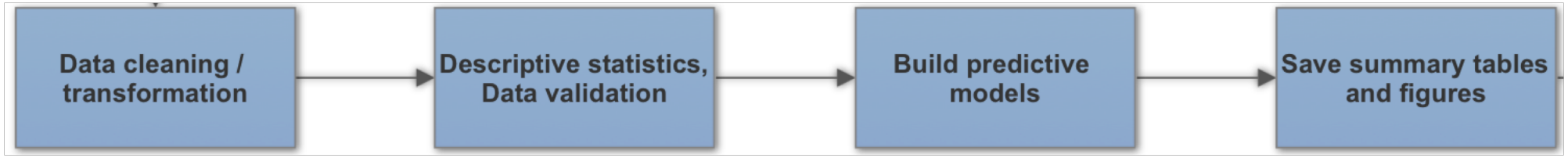
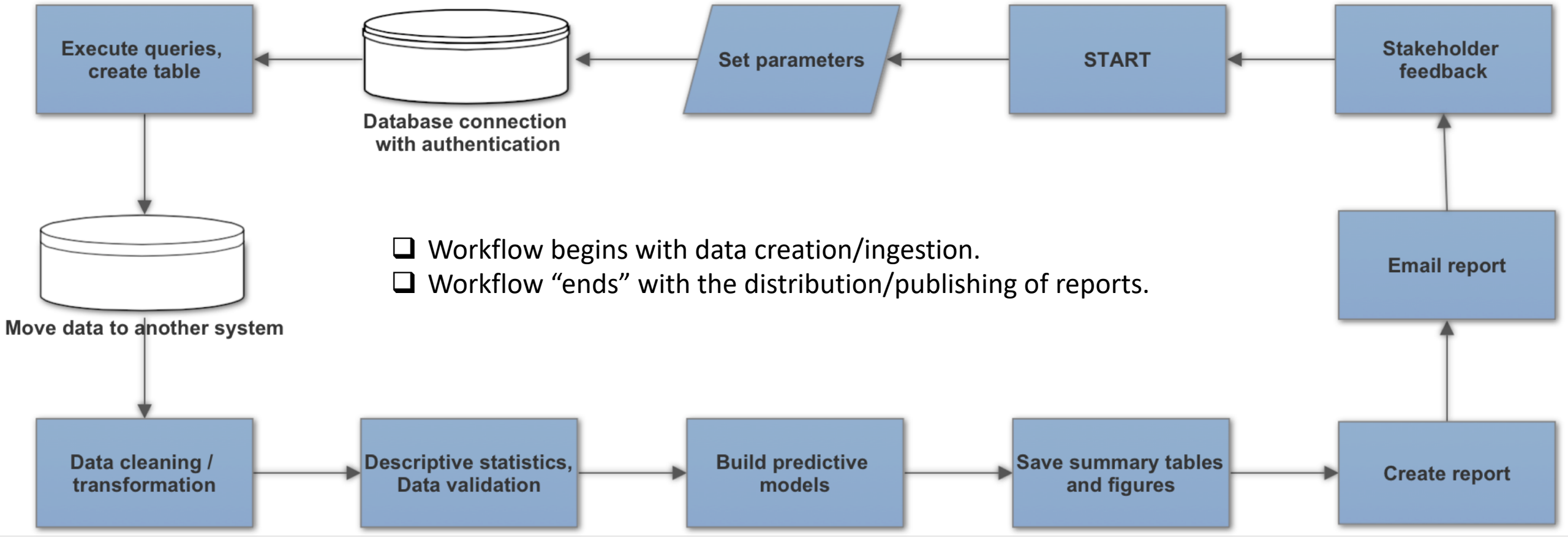
Data Scientist Workflow



Actual Data Scientist Workflow



- Workflow begins with data creation/ingestion.
- Workflow "ends" with the distribution/publishing of reports.

Automated Data Science Workflows

- An ***R*-bot** is an R script that executes one or more tasks in a data science workflow.
- Examples:
  - Data ingestion
  - Create report with dynamically generated content
  - Send emails
  - Version control
- An end-to-end automated data science workflow could consist of a collection of ***R-bots*** executed from a common framework.

Use Cases

- Well-defined analyses that will be performed over and over again
- Analyses in development stages, where feedback must be incorporated over and over again
- “Hands-free” automation
  - Task scheduler manages the runs
- “Manual” automation
  - Entire process kicks off as soon as the data scientist presses the button

Benefits

- Reproducible research
- Version control over entire process
- Less time spent on mundane, repetitive tasks
- Easier to get results reports generated and distributed to stakeholders

Workflow automation framework

- Adopt modularized approach, with flexibility to swap out components
- Use common framework from which all ***R-bots*** are executed (e.g., R, Bash)
- Set parameters (manually or dynamically)
- Re-use code (functions)
- Write code that creates/executes dynamically generated code
- Relinquish low level decisions to computer
  - Use conditional logic
  - Error handling
  - Automated validation of results

R packages for workflow management

- workflowr
- drake

```
library("workflowr")

# Configure Git (only need to do once per computer)
wflow_git_config(user.name = "Full Name", user.email = "email@domain")

# Start a new workflowr project
wflow_start("myproject")

# Build the site
wflow_build()

# Customize your site!
#   1. Edit the R Markdown files in analysis/
#   2. Edit the theme and layout in analysis/_site.yml
#   3. Add new or copy existing R Markdown files to analysis/

# Preview your changes
wflow_build()

# Publish the site, i.e. version the source code and HTML results
wflow_publish("analysis/*", "Start my new project")
```

Tools/Utilities

Task	R Packages	Bash Functions
Connect to SQL database, with authentication username/password; execute queries	RJDBC, odbc, RMySQL	--
Connect to Hadoop, with Kerberos authentication	krb5	kinit
Create/populate Excel spreadsheet	XLConnect	--
Generate reports (documents, html website)	rmarkdown, knitr	--
Email notifications, reports	mailR*, sendmailR*, gmailr+	mail/mailx
Schedule task to run at regular intervals	cronR	crontab

* More advanced configuration may be necessary in order to get these working behind firewalls with restricted network settings.

+ Works, but last major update was 2 years ago.

Enterprise considerations

- In enterprise setting, you may have limitations on which types of packages you can install on the server, so you may be limited to mostly base R or system commands.

- In the demo, I give an example of a workflow created under this scenario.

DEMO

Example is available in my public repository:

https://github.com/sydeaka/workflow-automation

DEMO: Instructions

- System requirements
  - Mac / Linux operating system
  - MYSQL (optional)
    - If you have MYSQL installed, set use_mysql=TRUE and create a credentials file in your system's home directory. The file should contain two lines:

```
username=YourUserName
password=YourPassword
```

    - If not, set use_mysql=FALSE to run without MYSQL
- To run
  - navigate to the top-level directory in the repository in your terminal
  - modify working directory at top of "mysql_example.sh" file
  - modify from/to email addresses in email.R, and create "gmail.txt" file in system home directory (file just contains your password as raw text, no quotes)
  - execute the following:

```
./mysql_example.sh
```

DEMO: Github directory structure

Folder	Subfolder	Contents
config		Session parameters, pointer to credential file location
data	dictionary	Lending Club data dictionary
	downloads	Downloaded zip files from Lending Club website + unzipped CSVs
	join_data	State-level datasets to be joined to Lending Club dataset
	modeling_data	Cleaned/transformed Lending Club data subset prepared for modeling
	sql	SQL scripts created/executed in the process
model_results		h2o model files + R workspace with objects saved for use in report
plots		Plots to be rendered in the report
R_bots		R-scripts executed in the workflow
reports		Rmarkdown files + rendered reports (HTML/Markdown formats)
slides		PPT and PDF of presentation
utils		Re-usable utilities that could be used in other projects

DEMO: Skeleton of `mysql_example.sh`

1. Read in MYSQL credentials and set session parameters
2. Download dataset from Lending Club website for selected year/quarter if it does not exist
3. Generate code that moves data into MYSQL database + join with existing dataset
4. Execute code created in #3
5. Generate code to create new MYSQL table with selected attributes for modeling
6. Execute code created in #5
7. Pull MYSQL modeling table into an R session, apply transformations
8. Build predictive models and save results
9. Create report of descriptive stats + modeling results
10. Email report
11. Check workflow code into Github repository

Other considerations

- Software, package, platform dependencies (Ex. Spark 2.0 vs 2.2; h2o 3.14 vs 3.18); solution: environments
- Storage space and memory requirements
- Scale: if dataset gets larger over time, the solution might not work as well (scale up). May need to adjust framework on the front end or do it later. Monitor strain on resource demands, run time, and other metrics
- Tech dev requirements if you want to move process to production
- Documentation of the workflow
- Redundancy: make sure more than one person understands the process well and can help maintain it

THANKS!