Using R for Scalable Data Science

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Microsoft Corporation

Acknowledgements: Gopi Kumar, Paul Shealy, Katherine Zhao

KDD 2017
Halifax, NS

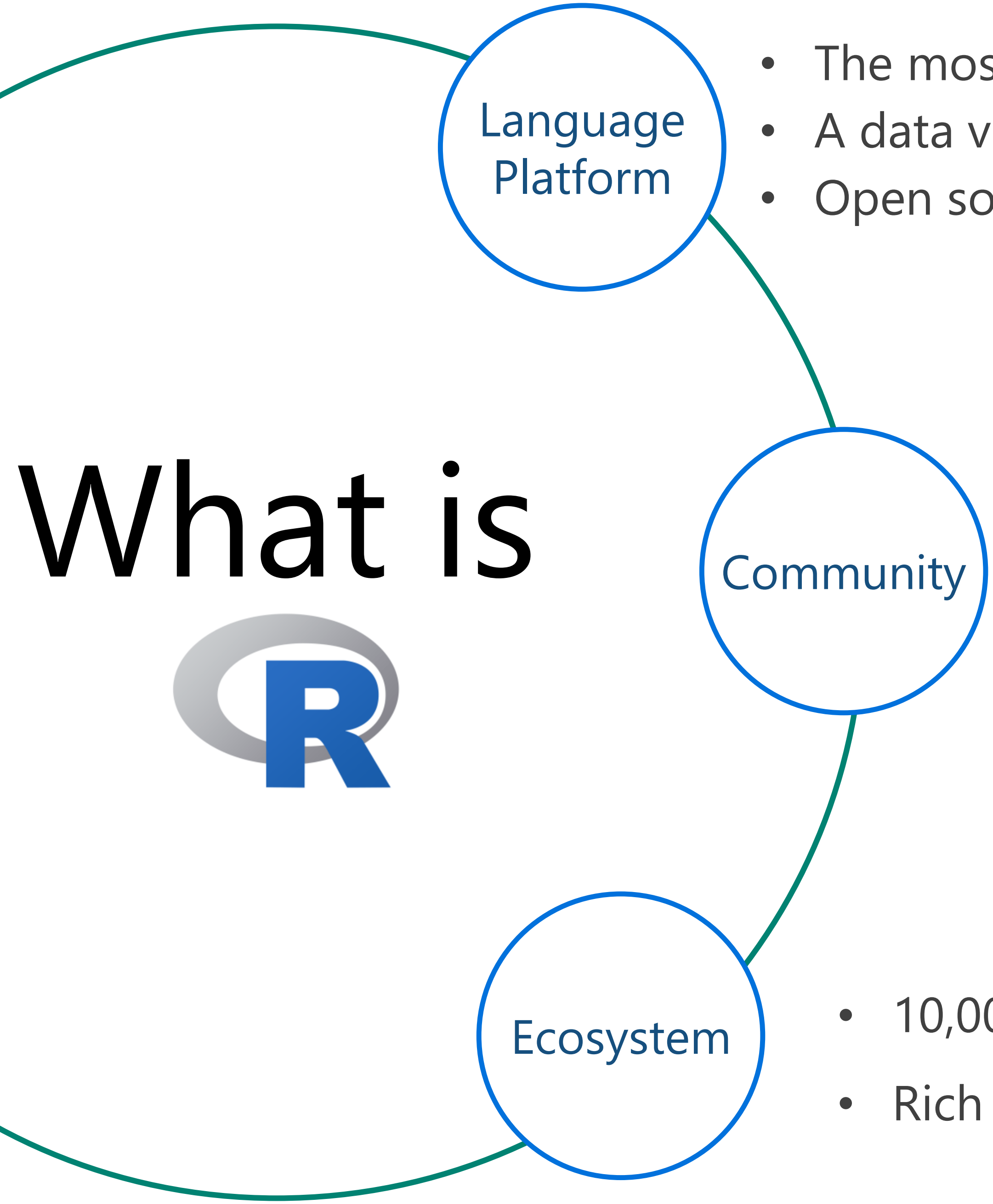
TUTORIAL MATERIAL & SLIDES:

https://aka.ms/kdd2017r

Tutorial Outline

- Introduction to R for Scalable Data Science
- R in SQL Server
- R in Apache Spark
- Distributed model training and parameter optimization use cases
  - Learning Curves: Detecting Gibberish
  - Grouped Time Series Forecasting
- Sentiment Analysis with Pretrained Deep Learning Model

What is R



Language Platform

- The most popular statistical programming language
- A data visualization tool
- Open source

Community

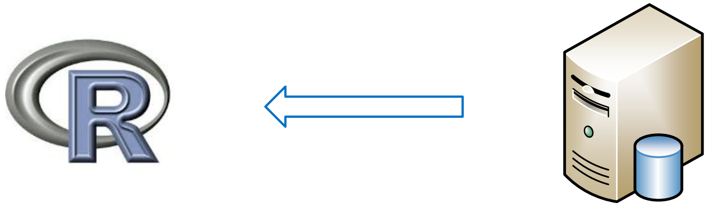
- 2.5+M users
- Taught in most universities
- Many common use cases across industry
- Thriving user groups worldwide
  - 5th in 2016 IEEE Spectrum rank
  - 42% pro analysts prefer R (highest amongst R, SAS, python)

Ecosystem

- 10,000+ contributed packages
- Rich application & platform integration

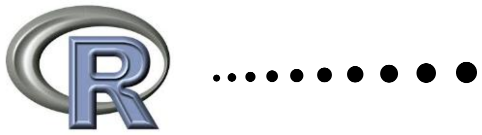
Challenges with Embracing Open Source R

Data Movement



Moving data from the database to the R Runtime becomes painful as data volumes grow and carries security risks

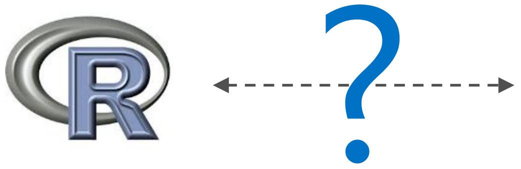
Scale/Performance



Document_Ty...	Sell_to_Custo...	Document_No	No	Quantity	Amount
Order	38008	181005	1920-S	4	1597.52
Order	38128456	181009	1976-W	5	444155.4
Order	38128456	181009	1964-W	2	282566.78
Order	43687129	181011	1920-S	5	3847.26
Order	43687129	181011	1990-S	12	2176.28
Order	43687129	181011	1996-S	1	1314.44

R runs single threaded and only accommodates datasets that fit into available memory

Operationalization



Sales Predictions

How do I call the R script from my production application?

Scalable R Solutions

- R packages for scaling on single machines
  - The **`bigmemory`** project
  - **`ff`** and related packages
  - **`foreach`** with **`doParallel`**

- R packages for scaling with distributed computing
  - **`SparkR`**
  - **`sparklyr`**
  - **`RevoScaleR`** (Microsoft R Server)
  - **`h2o,rsparkling`**
  - **`foreach`** with **`doAzureParallel`**, **`doSNOW`**

SQL Server R Services

Reduce or eliminate data movement with In-Database analytics

- SQL Server 2016 extensibility mechanism allows secure execution of R scripts on the SQL Server

Operationalize R scripts and models

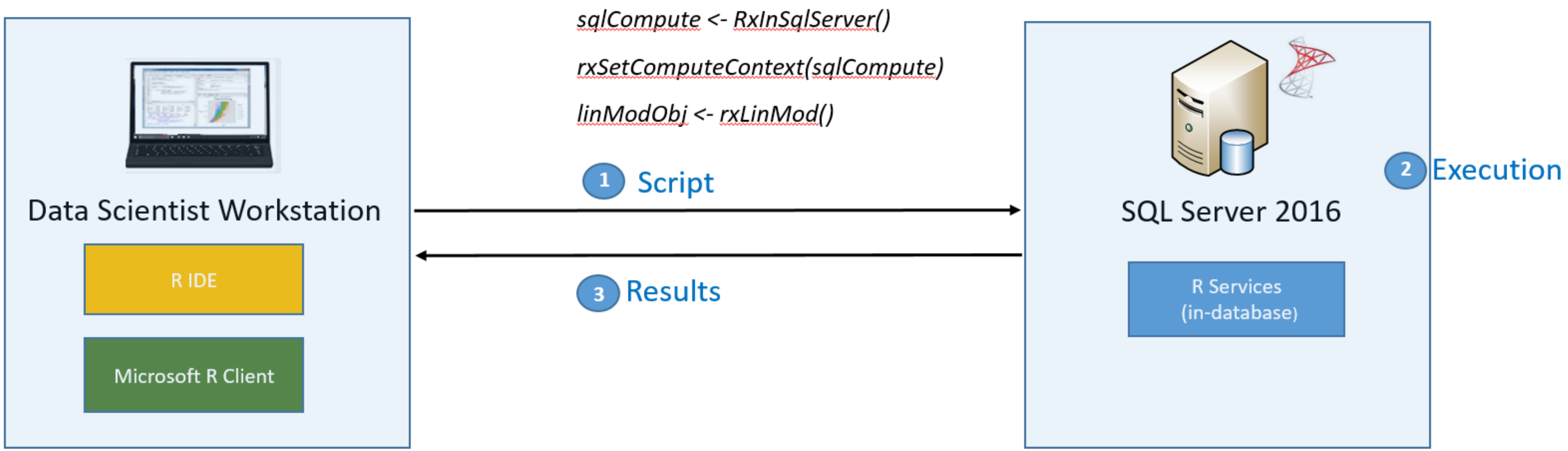
- Use familiar T-SQL stored procedures to invoke R scripts from your application
- Embed the returned predictions and plots in your application

Enterprise Performance and scale

- Use SQL Server's in-memory querying and Columnstore Indexes
- Leverage RevoScaleR support for large datasets and parallel algorithms
- Easily deploy to Spark cluster by just changing compute context

R Services in-database: Data Exploration and Predictive Modeling (‘Data Scientist’)

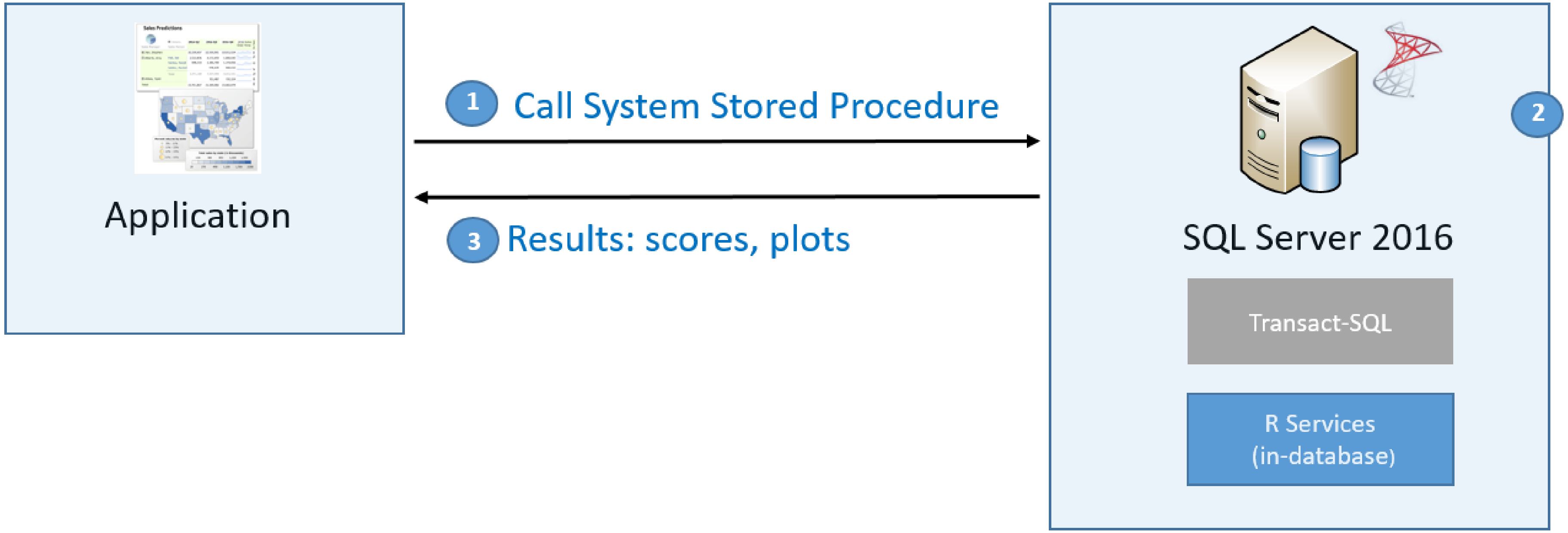
Working from my R IDE on my workstation, I can execute an R script that runs in-database, and get the results back.



```
sqlCompute <- RxInSqlServer()
rxSetComputeContext(sqlCompute)
linModObj <- rxLinMod()
```

R Services in-database: Operationalizing R Code via T-SQL (‘Developer’)

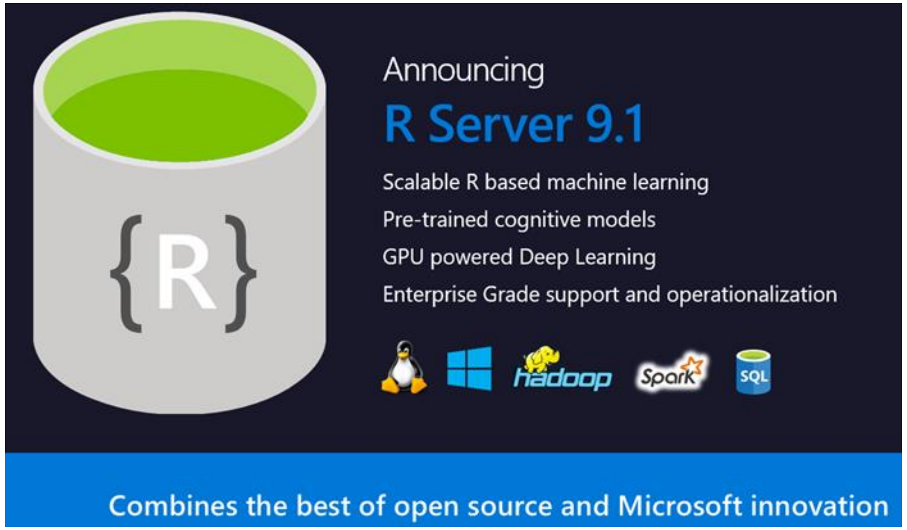
I can call a T-SQL System Stored Procedure from my application and have it trigger R script execution in-database. Results are then returned to my application (predictions, plots, etc).



The stored procedure contains R code and executes in-database.

```
exec sp_execute_external_script
  @ languague = ‘R’
,  @script =
-- R code --
```

Free Developer's Versions Available



Announcing

R Server 9.1

Scalable R based machine learning

Pre-trained cognitive models

GPU powered Deep Learning

Enterprise Grade support and operationalization

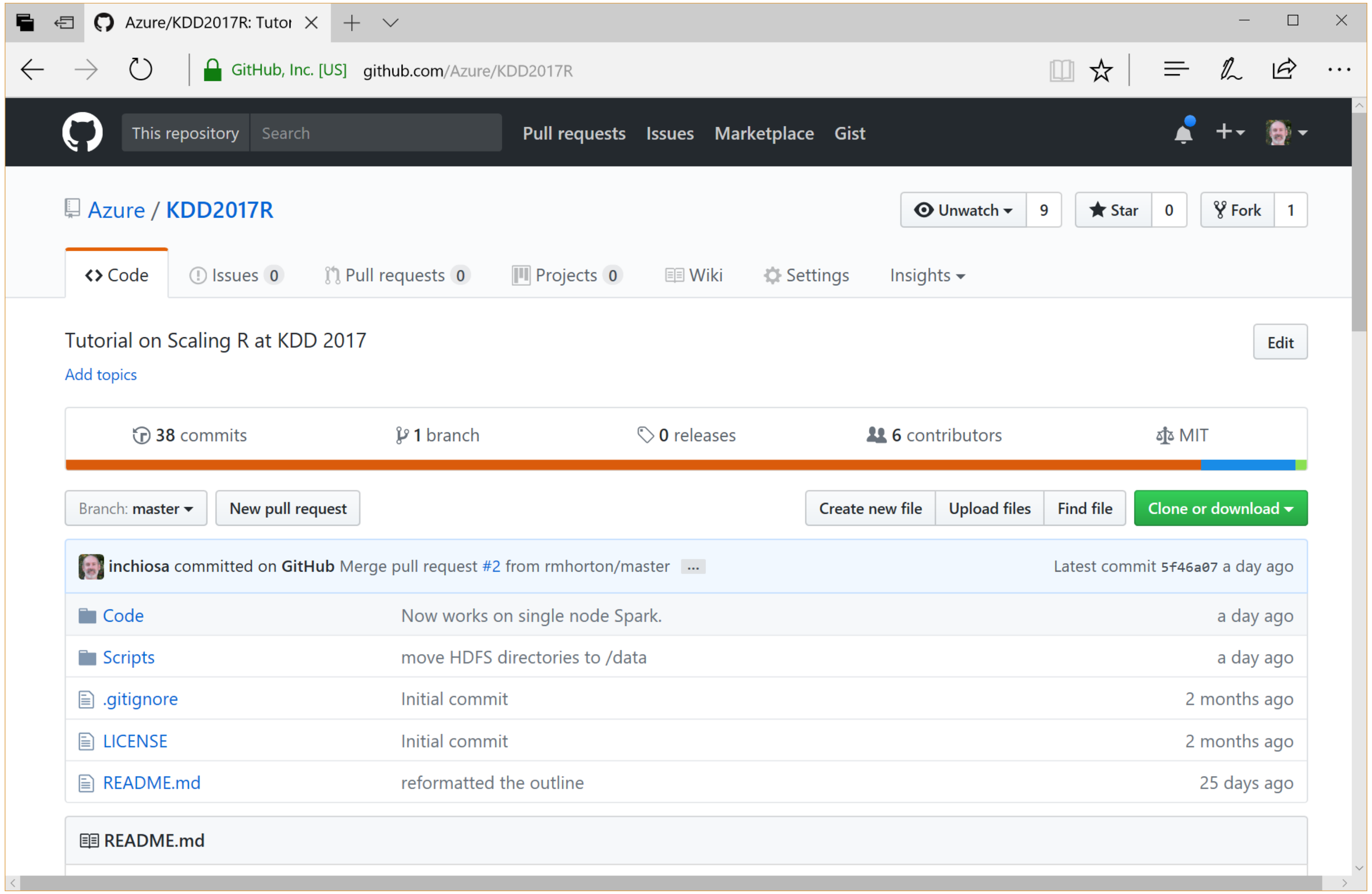
Combines the best of open source and Microsoft innovation

https://aka.ms/freemrs

Microsoft® SQL Server®

https://aka.ms/sqlserverdeveloper

GitHub repository for all code and scripts



Azure / KDD2017R

Tutorial on Scaling R at KDD 2017

38 commits · 1 branch · 0 releases · 6 contributors · MIT

inchiosa committed on GitHub Merge pull request #2 from rmhorton/master … Latest commit 5f46a07 a day ago

Code	Now works on single node Spark.	a day ago
Scripts	move HDFS directories to /data	a day ago
.gitignore	Initial commit	2 months ago
LICENSE	Initial commit	2 months ago
README.md	reformatted the outline	25 days ago

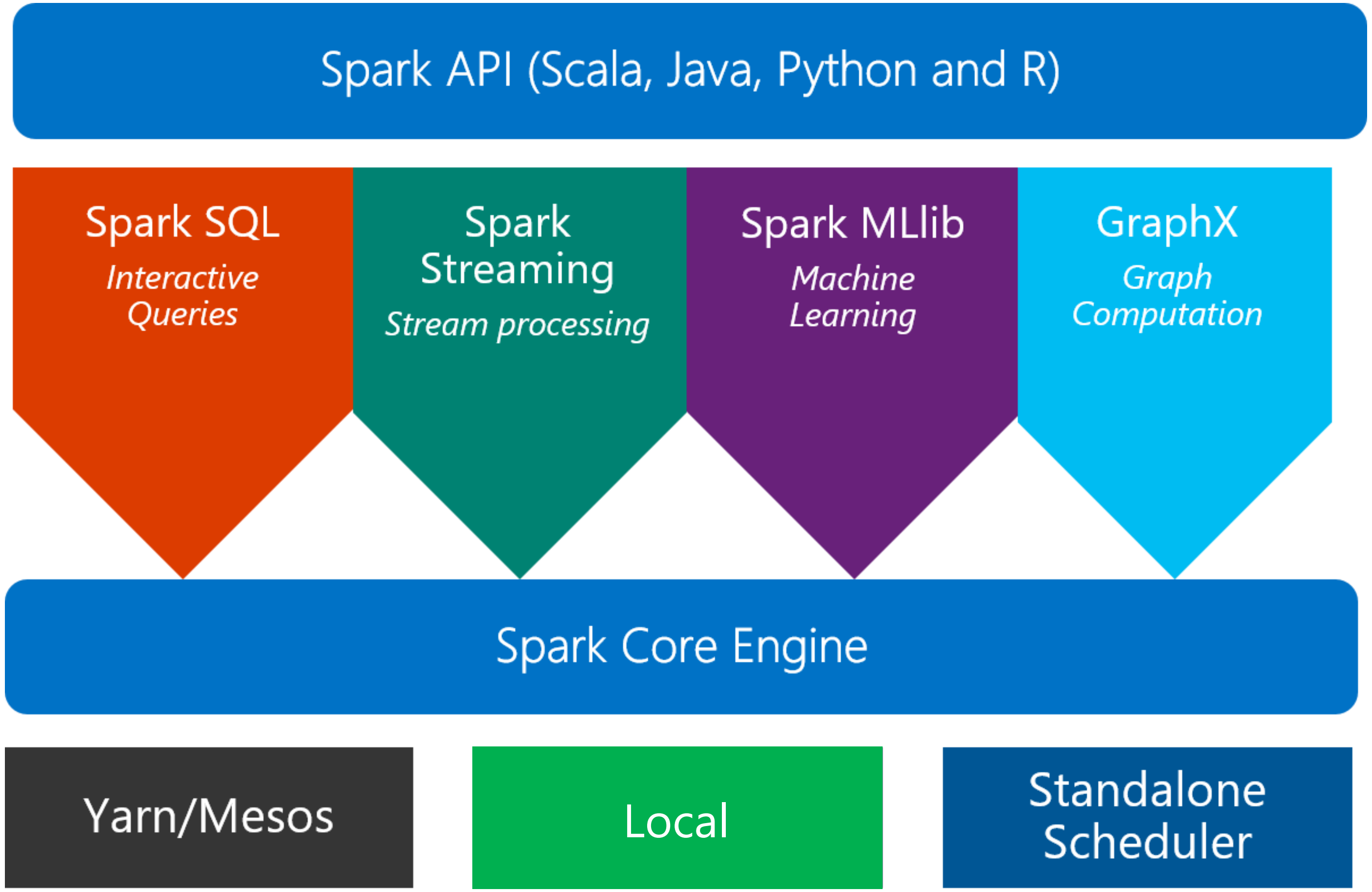
https://aka.ms/kdd2017r

Distributed computing on Spark

Brief intro to Spark, its APIs and OS R packages

Scaling R on Spark Clusters

- What is Spark?
  - An unified, open source, parallel, data processing framework for Big Data Analytics



Spark API (Scala, Java, Python and R)

Spark SQL *Interactive Queries*

Spark Streaming *Stream processing*

Spark MLlib *Machine Learning*

GraphX *Graph Computation*

Spark Core Engine

Yarn/Mesos

Local

Standalone Scheduler

`SparkR`: R API included with Apache Spark

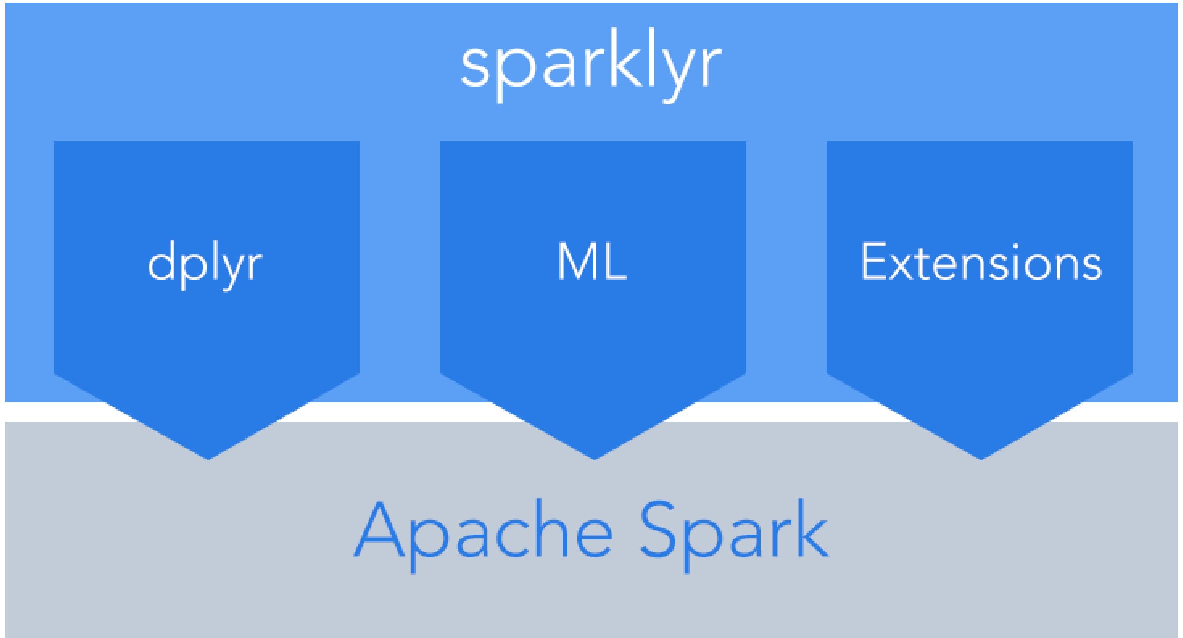
- An R package provides a light-weight frontend to use Apache Spark from R and allows data scientists to analyze large datasets.
- **`SparkDataFrame`** is distributed collection of data organized into named columns.
- **`SparkR`** can create `SparkDataFrames` from local R data frames, csv, json and parquet files.
- Access tables from **`Hive`** MetaStore.
- Pre-configured on Spark clusters in Azure HDInsight.

Data processing and modeling with SparkR

- Supports functions for processing structured data
  - *Selections*: select(), filter()
  - *Grouping, Aggregations*: summarize(), arrange()
  - *Running local R functions distributed*: spark.lapply()
  - *Applying UDFs on each partition/group of a SparkDataFrame*: dapply(), dapplyCollect(), gapply(), gapplyCollect()

- Uses **`MLlib`** to train models and allows model persistence
  - Generalized Linear Model
  - Survival regression
  - Naive Bayes
  - KMeans
  - Logistic Regression
  - Gradient Boosted Tree
  - Random Forest
  - … others

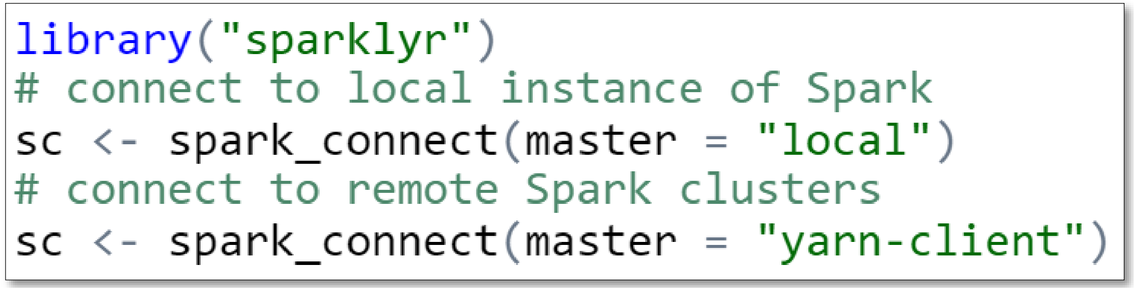
sparklyr: R interface for Apache Spark



- Easy installation from CRAN

```
install.packages("sparklyr")
```

- Connect to both local instances of Spark and remote Spark clusters



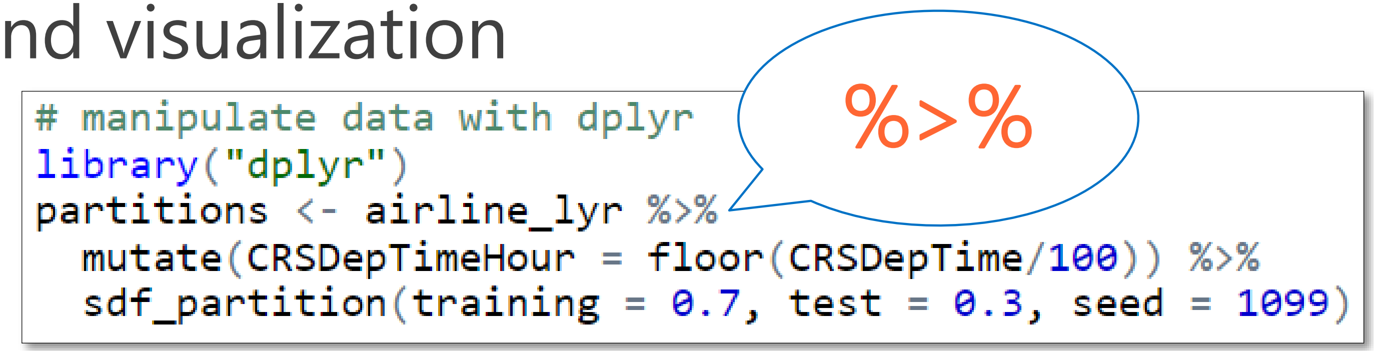
```
library("sparklyr")
# connect to local instance of Spark
sc <- spark_connect(master = "local")
# connect to remote Spark clusters
sc <- spark_connect(master = "yarn-client")
```

- Loads data into **`SparkDataFrame`** from: local R data frames, Hive tables, CSV, JSON, and Parquet files.

Source: http://spark.rstudio.com/

dplyr and ML in sparklyr

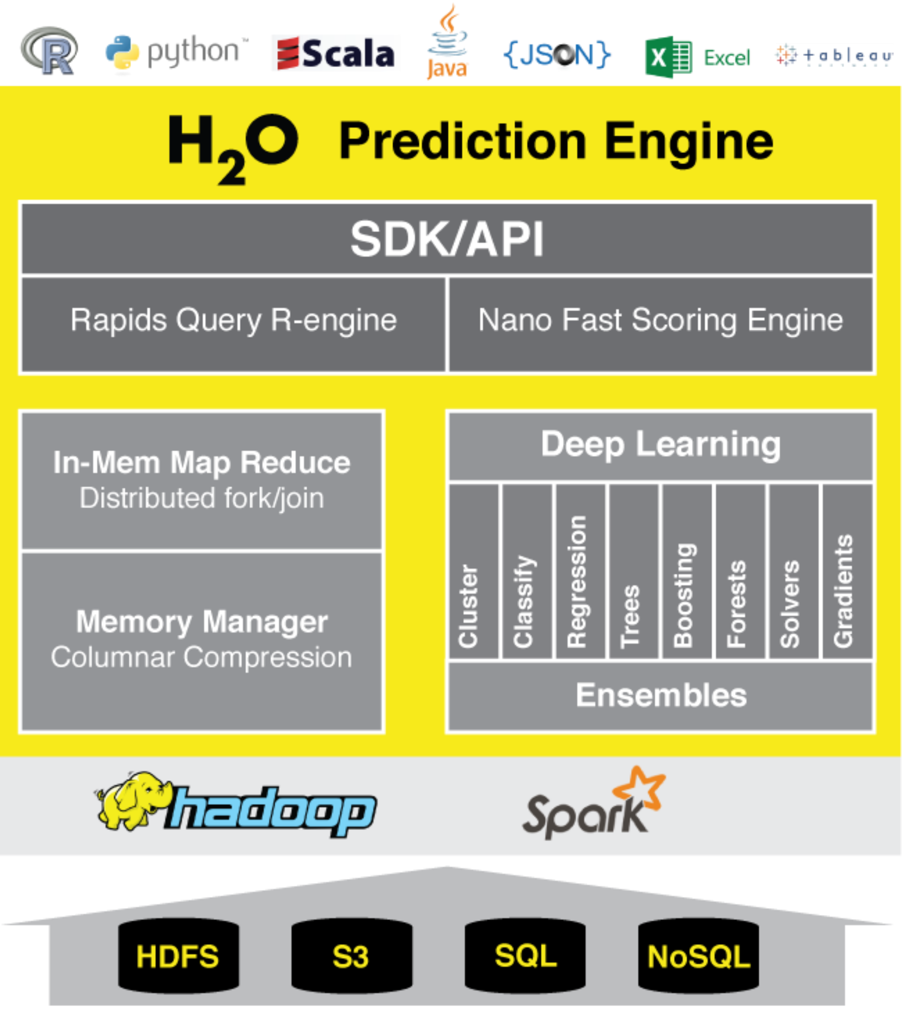
- Provides a complete **dplyr** backend for data manipulation, analysis and visualization



```
# manipulate data with dplyr
library("dplyr")
partitions <- airline_lyr %>%
  mutate(CRSDepTimeHour = floor(CRSDepTime/100)) %>%
  sdf_partition(training = 0.7, test = 0.3, seed = 1099)
```

- Includes 3 family of functions for machine learning pipeline
  - **ml_***: Machine learning algorithms for analyzing data provided by the spark.ml package.
    - K-Means, GLM, LR, Survival Regression, DT, RF, GBT, PCA, Naive-Bayes, Multilayer Perceptron, LDA
  - **ft_***: Feature transformers for manipulating individual features.
  - **sdf_***: Functions for manipulating SparkDataFrames.

h2o: prediction engine in R



http://www.h2o.ai/product/

- Optimized for “in memory” processing of distributed, parallel machine learning algorithms on clusters.

- **Data manipulation and modeling on H2OFrame**: R functions + `h2o` pre-fixed functions.
  - *Transformations*: h2o.group_by(), h2o.impute()
  - *Statistics*: h2o.summary(), h2o.quantile(), h2o.mean()
  - *Algorithms*: h2o.glm(), h2o.naiveBayes(), h2o.deeplearning(), h2o.kmeans()

- `rsparkling` package: h2o on Spark
  - Provides bindings to `h2o`’s machine learning algorithms
  - Simple data conversion: SparkDataFrame -> H2OFrame

R Server 9.1: Scale-out R, Enterprise-Class Support

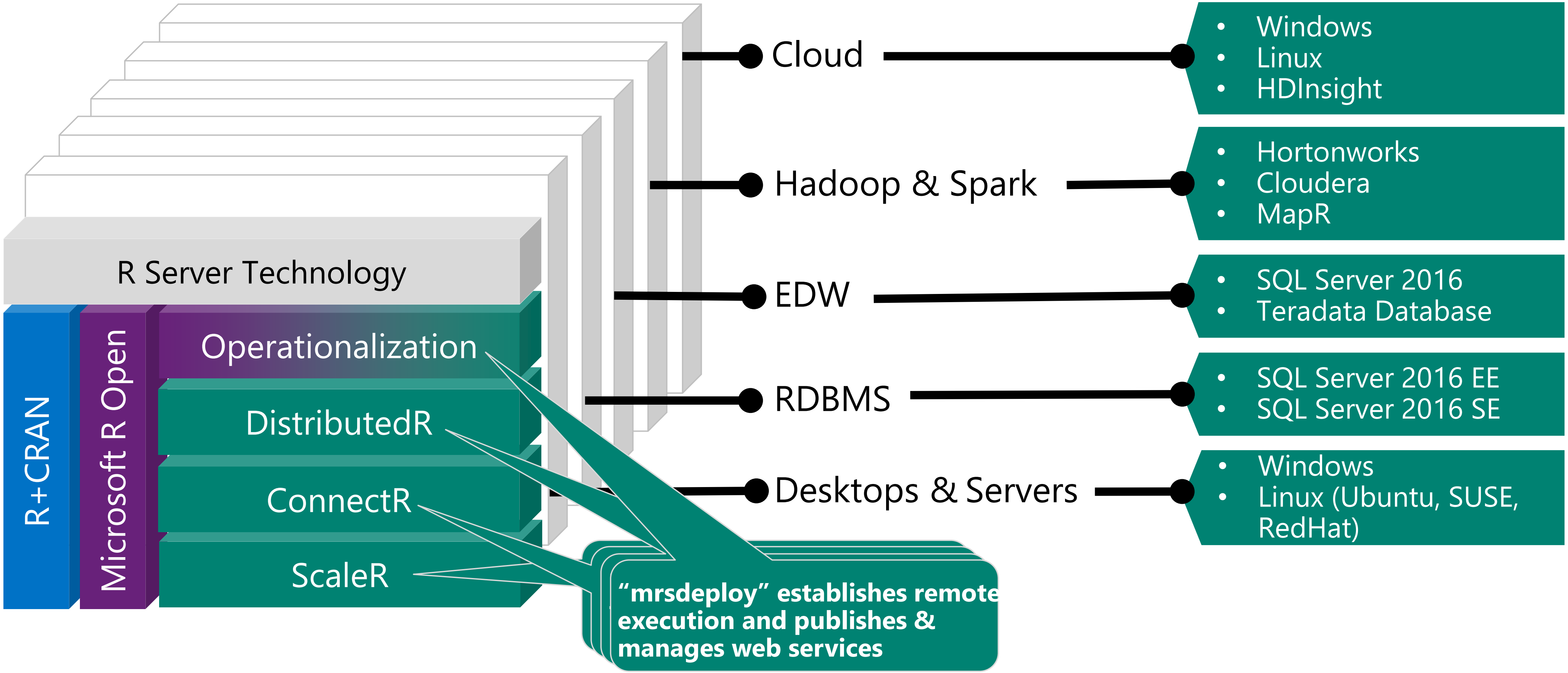
- 100% compatible with open source R
  - Virtually any code/package that works today with R will work in R Server.

- Ability to parallelize any R function
  - Ideal for parameter sweeps, simulation, scoring.

- Wide range of scalable and distributed **`rx`** pre-fixed functions in **`RevoScaleR`** package.
  - *Transformations*: rxDataStep()
  - *Statistics*: rxSummary(), rxQuantile(), rxChiSquaredTest(), rxCrossTabs()…
  - *Algorithms*: rxLinMod(), rxLogit(), rxKmeans(), rxBTrees(), rxDForest()…
  - *Parallelism*: rxSetComputeContext()

- ML featurizers and algorithms in **`MicrosoftML`** package

RevoScaleR: Portable across multiple platforms



- Windows
- Linux
- HDInsight

- Hortonworks
- Cloudera
- MapR

- SQL Server 2016
- Teradata Database

- SQL Server 2016 EE
- SQL Server 2016 SE

- Windows
- Linux (Ubuntu, SUSE, RedHat)

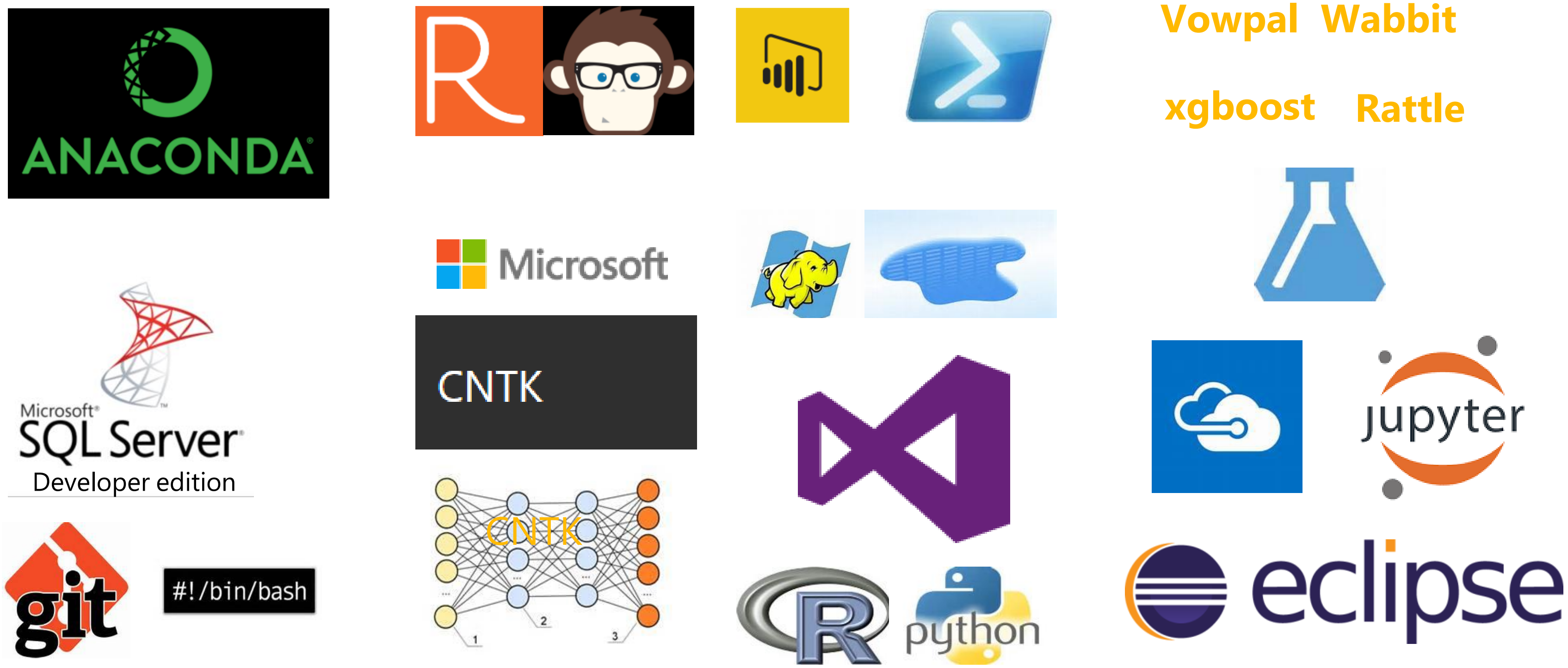
“mrsdeploy” establishes remote execution and publishes & manages web services

Hands-on Tutorial:
Airline Arrival Delay Prediction using R Server and sparklyr

Mario Inchiosa

Azure Data Science Virtual Machine (Ubuntu Linux)

Data-science virtual machine



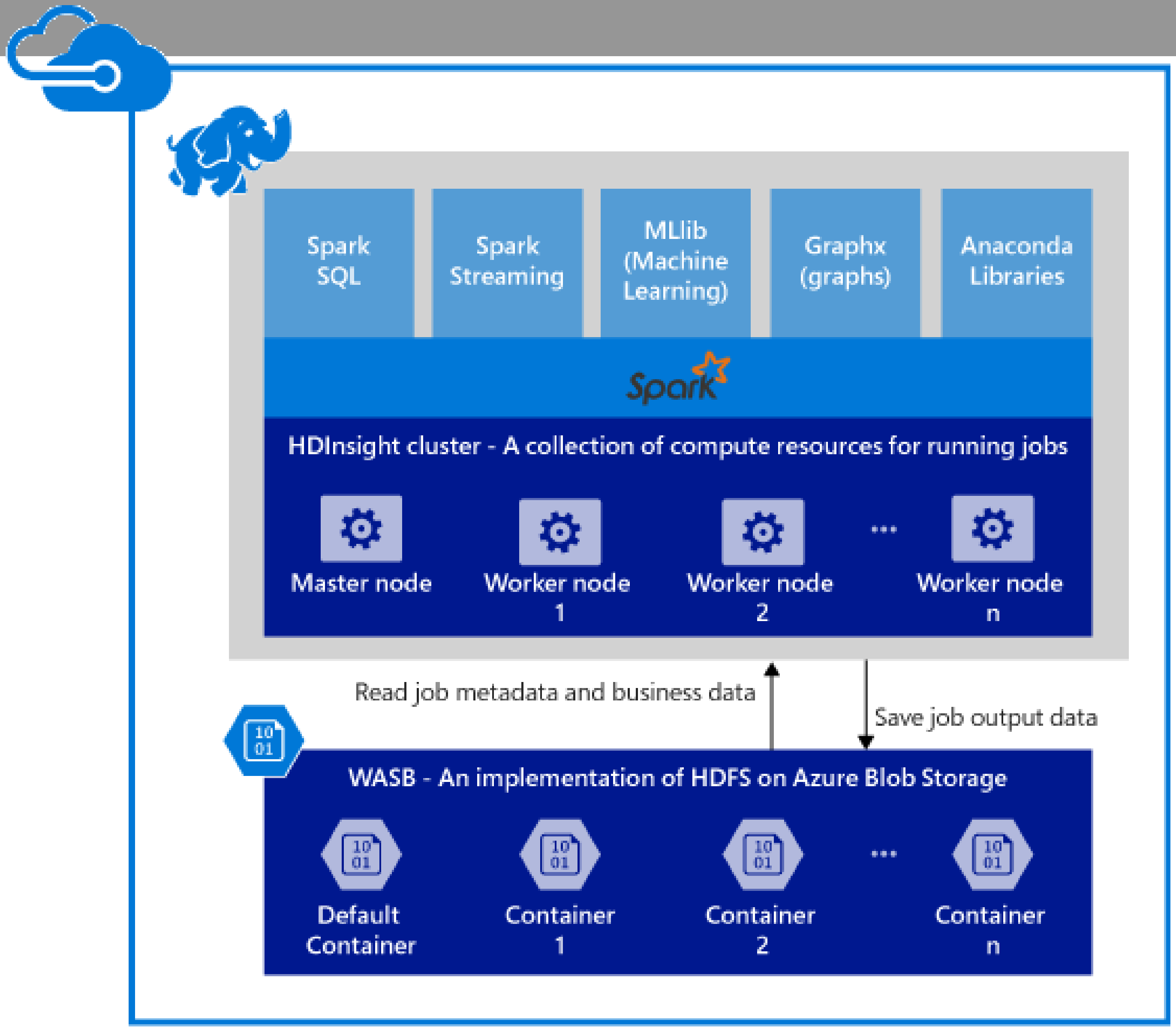
Vowpal Wabbit

xgboost Rattle

- Spark 2.1.1
- HDFS
- YARN

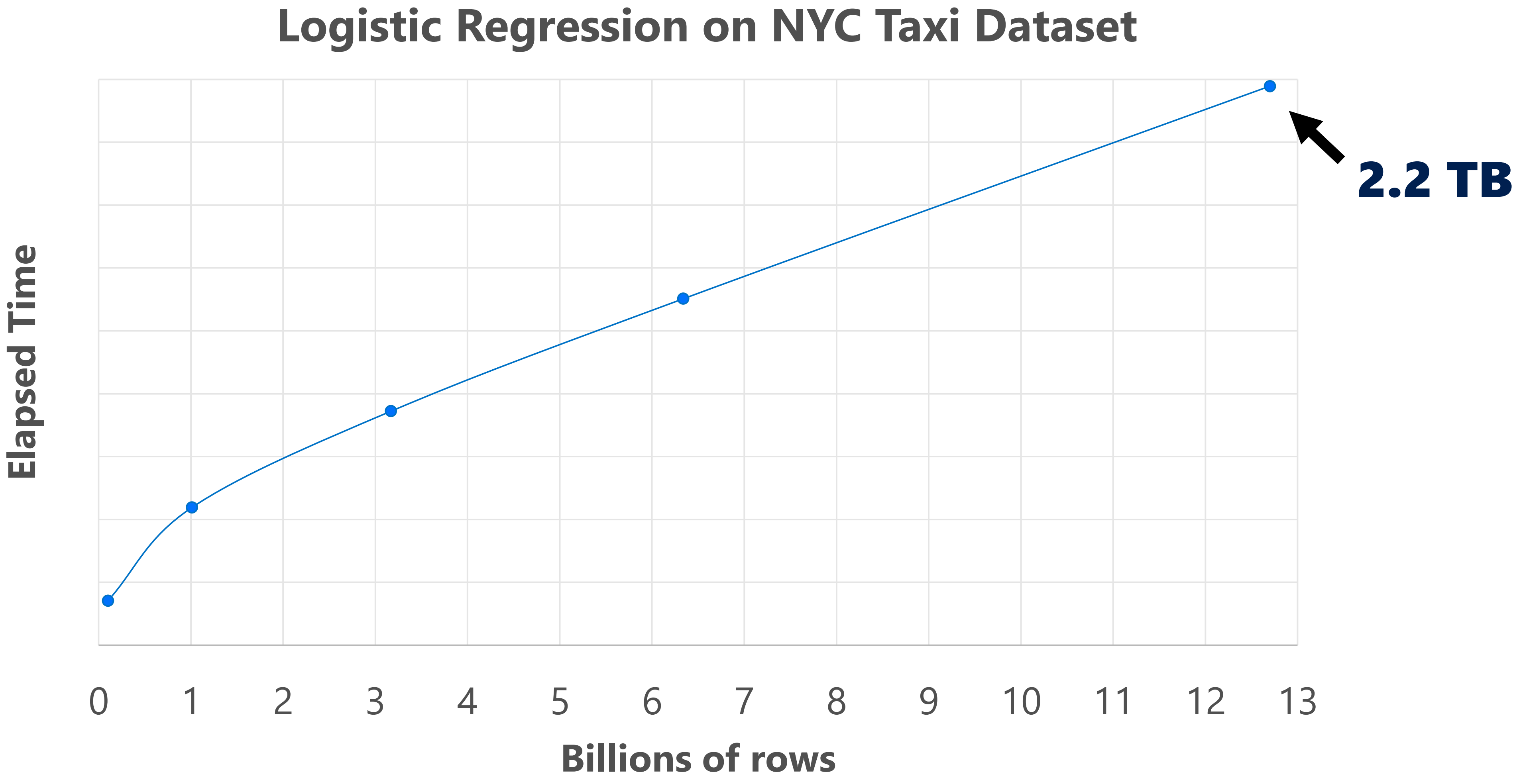
http://aka.ms/dsvm

Spark R Server Clusters in Azure HDInsight



- Provisions Azure compute resources with Spark and R Server installed and configured
- Supports multiple versions of Spark and R Server
- Stores data in Azure Blob storage (WASB), Azure Data Lake Store or Local HDFS.

R Server on Hadoop/HDInsight scales to hundreds of nodes, billions of rows and terabytes of data



Airline Arrival Delay Prediction in Spark

- Clean/Join – sparklyr
- Train/Score/Evaluate – RevoScaleR
- Deploy/Consume – mrsdeploy

Airline data set

- Passenger flight on-time performance data from the US Department of Transportation’s TranStats data collection
- >20 years of data
- 300+ Airports
- Every carrier, every commercial flight
- http://www.transtats.bts.gov

Weather data set

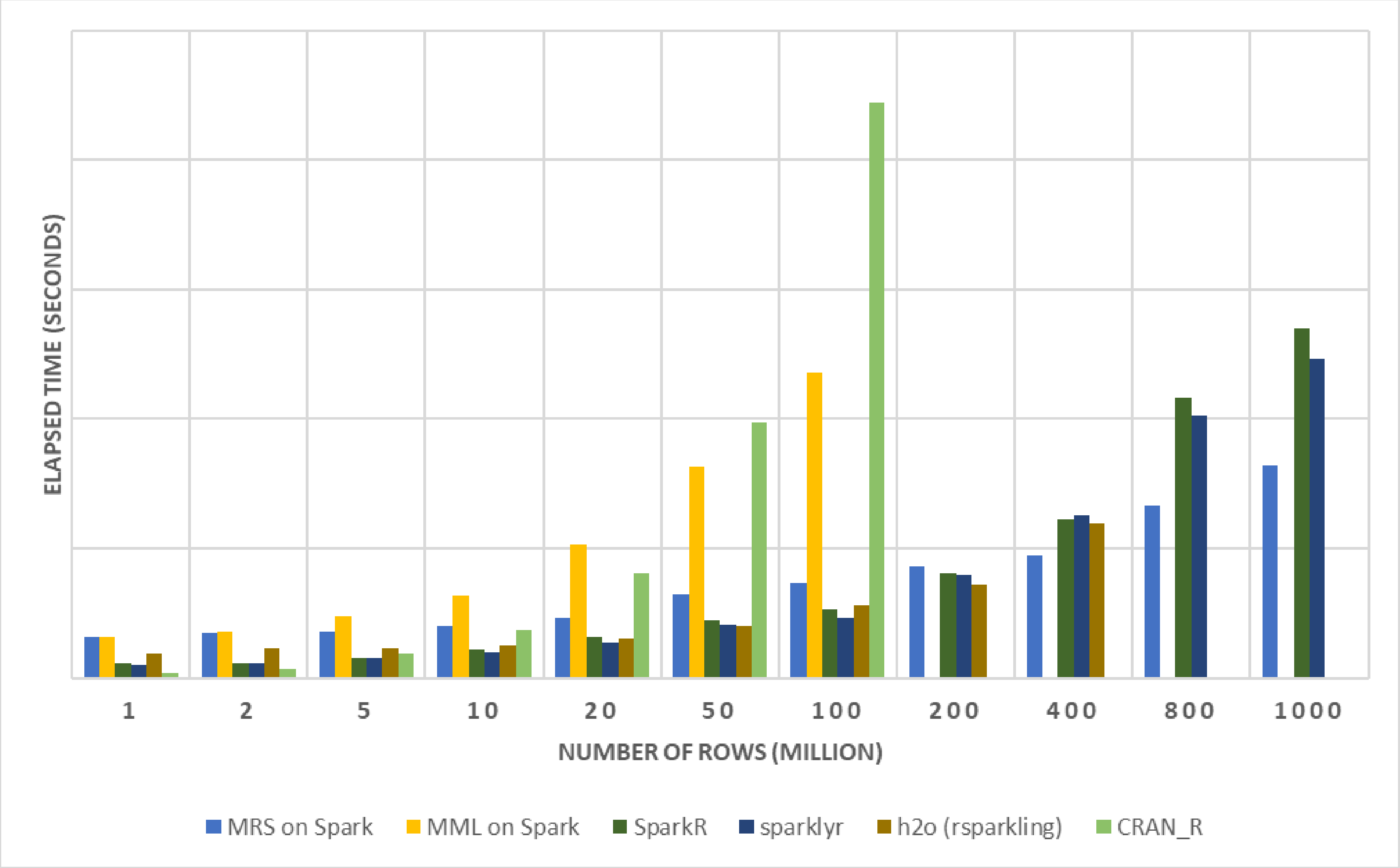
- Hourly land-based weather observations from NOAA
- > 2,000 weather stations
- http://www.ncdc.noaa.gov/orders/qclcd/

Comparisons

Base and scalable approaches comparison

Approach	Scalability	Spark	MapReduce	SQL Server	Teradata
Base R	Single machines				
SparkR	Single + Distributed computing	X			
sparklyr	Single + Distributed computing	X			
h2o	Single + Distributed computing	X	X		
RevoScaleR	Single + Distributed computing	X	X	X	X

R Server on Spark - faster and more scalable



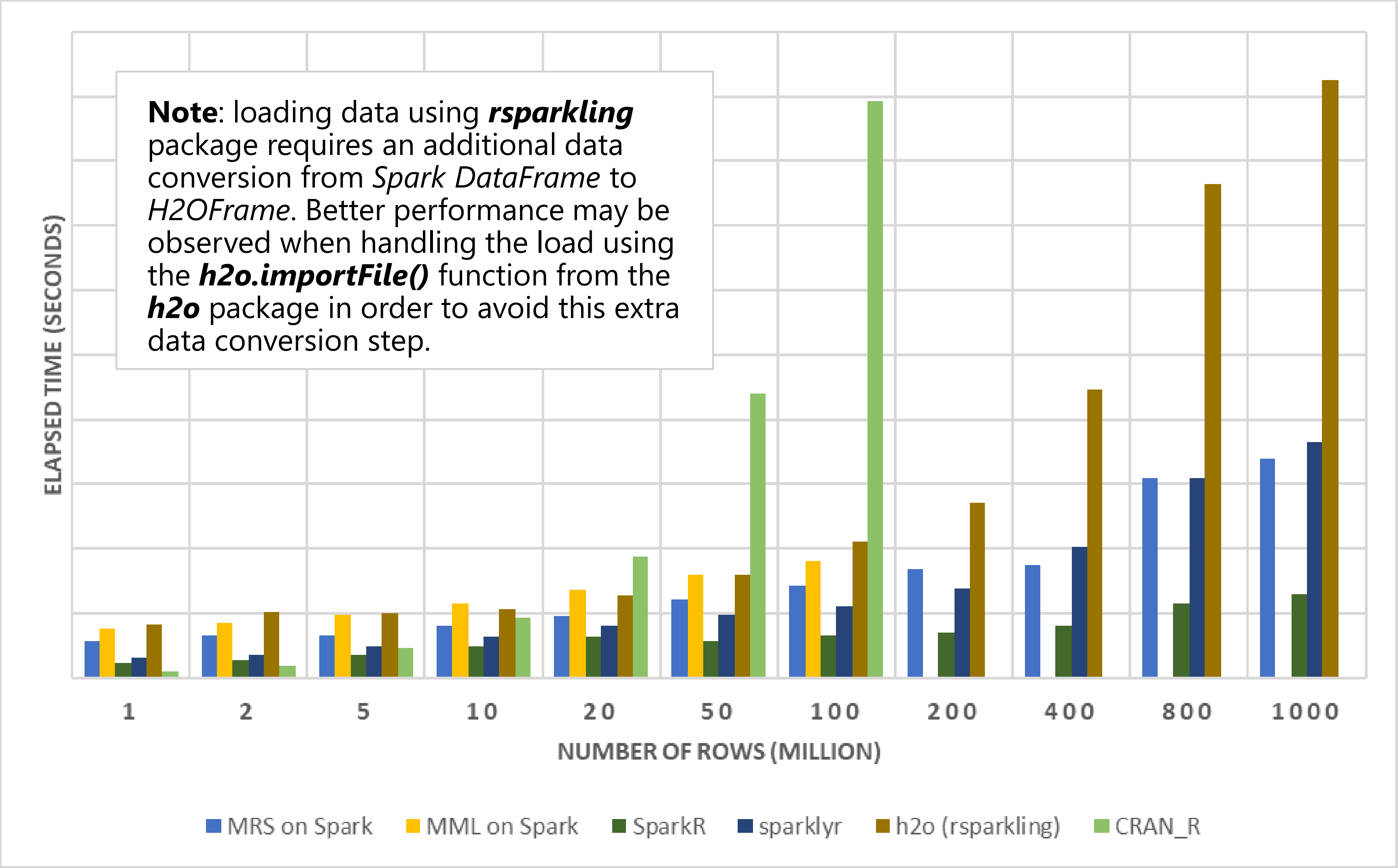
End-to-End Process:

- Load Data from .csv
- Transform Features
- Split Data: Train + Test
- Fit Model: Logistic Regression
- Predict and Write Outputs

Configuration:

- 1 Edge Node: 16 cores, 112GB
- 4 Worker Nodes: 16 cores, 112GB
- Dataset: Duplicated Airlines data (.csv)
- Number of columns: 26

Fastest loading data: SparkR



Note: loading data using ***rsparkling*** package requires an additional data conversion from *Spark DataFrame* to *H2OFrame*. Better performance may be observed when handling the load using the ***h2o.importFile()*** function from the ***h2o*** package in order to avoid this extra data conversion step.

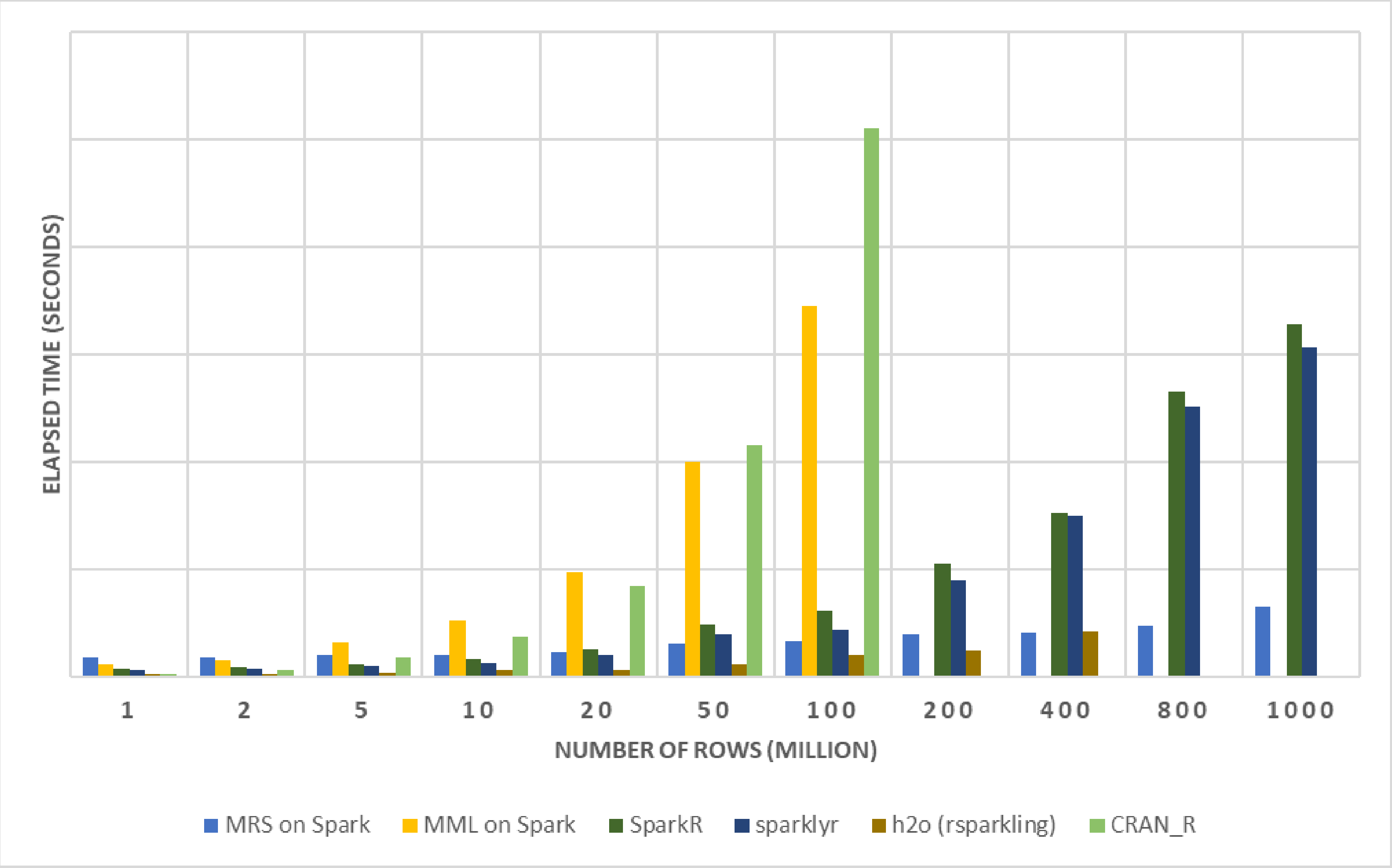
Load Data:

- MRS on Spark: **XDF**
- MML on Spark: **XDF**
- SparkR: **Spark DF**
- sparklyr: **Spark DF**
- h2o: **H2OFrame**
- CRAN R: **DF**

Configuration:

- 1 Edge Node: 16 cores, 112GB
- 4 Worker Nodes: 16 cores, 112GB
- Dataset: Duplicated Airlines data (.csv)
- Number of columns: 26

Fastest fitting big data: R Server



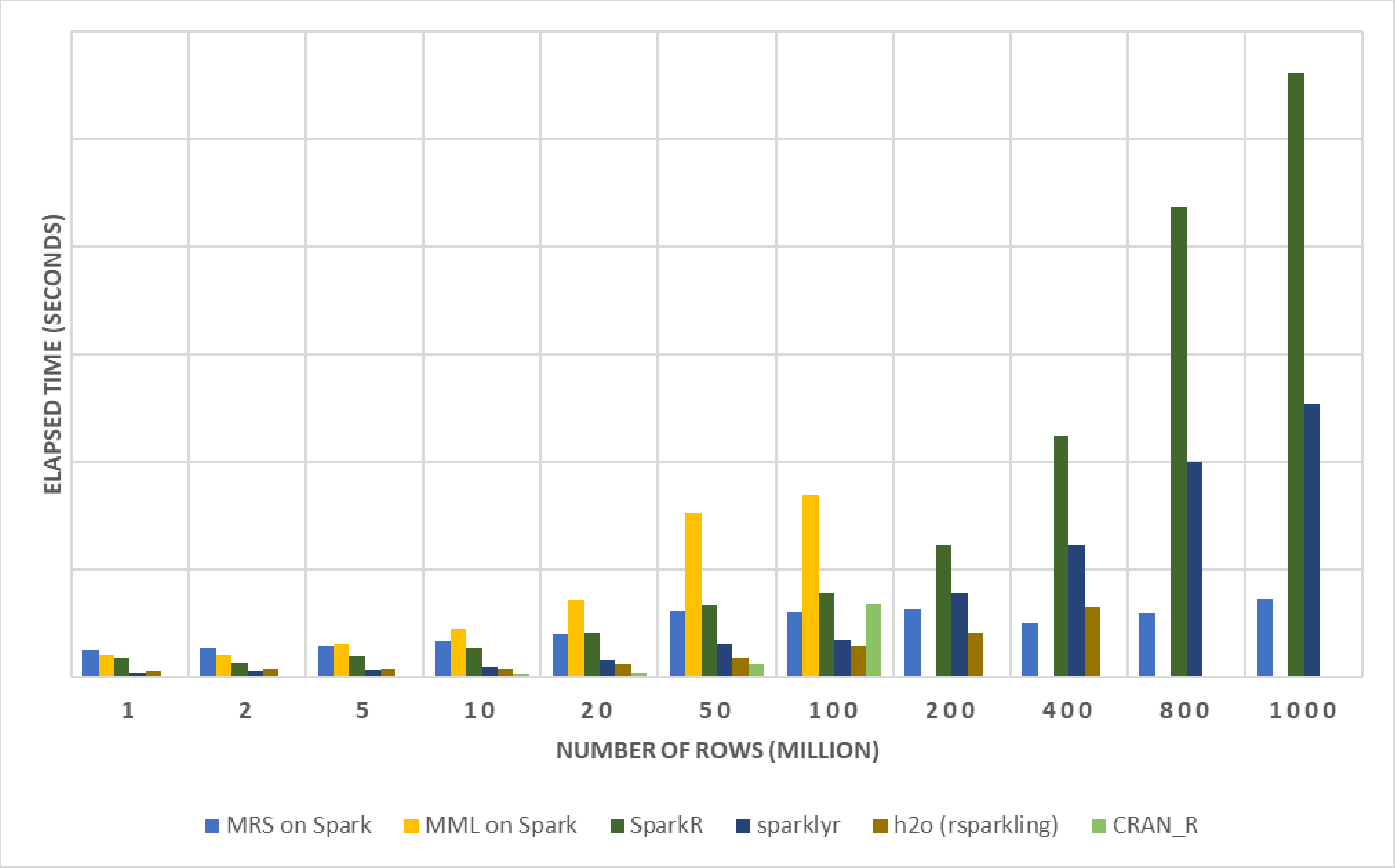
Fit model:

- Logistic regression

Configuration:

- 1 Edge Node: 16 cores, 112GB
- 4 Worker Nodes: 16 cores, 112GB
- Dataset: Duplicated Airlines data (.csv)
- Number of columns: 26

Fastest making predictions: R Server



Predict:

- Outputs predictions into files in HDFS

Configuration:

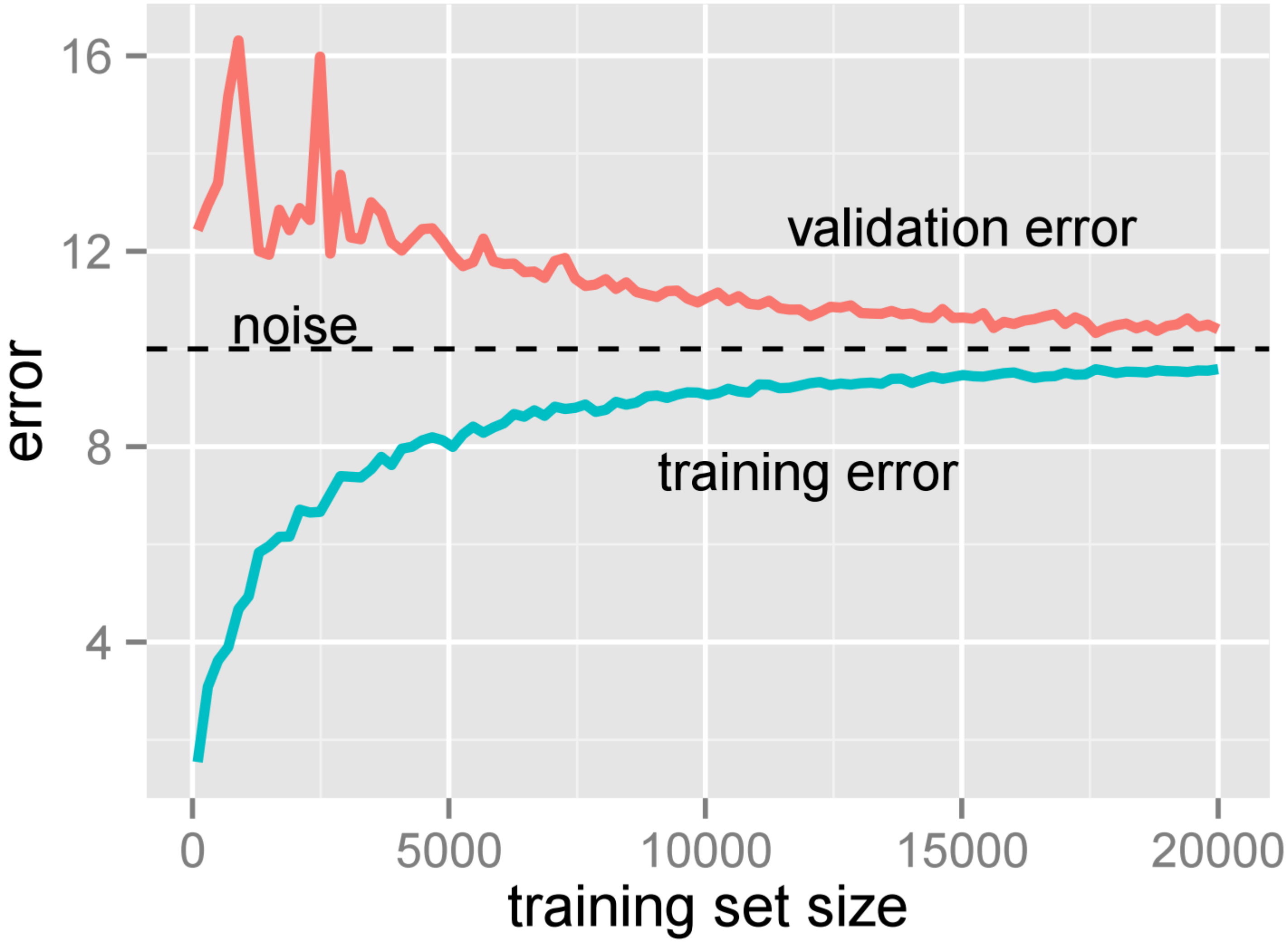
- 1 Edge Node: 16 cores, 112GB
- 4 Worker Nodes: 16 cores, 112GB
- Dataset: Duplicated Airlines data (.csv)
- Number of columns: 26

Distributed model training and parameter optimization:

Learning Curves on Big Data

Robert M. Horton, PhD MS
Senior Data Scientist

Learning Curve



Detecting Gibberish

Was the value entered on a web form a real name?

Training Set

real: unique names from babynames database (71323)

pseudogibberish: simulated keymash (712625)

random: randomly sampled lower case letters (712695)

```
         name        category is_real
1     UIOPUIO pseudogibberish   FALSE
2      A|A|SD pseudogibberish   FALSE
3   nvsfmxnkw          random   FALSE
4        jbhu          random   FALSE
5      ethjef          random   FALSE
6     opndgsc          random   FALSE
7        smly          random   FALSE
8    ASDASDAS pseudogibberish   FALSE
9       sbzjo          random   FALSE
10     ellqnc          random   FALSE
11   rererеuy pseudogibberish   FALSE
12      uswfs          random   FALSE
13   tztxksfl          random   FALSE
14      DSA|} pseudogibberish   FALSE
15     Kaylah            real    TRUE
16     rewrew pseudogibberish   FALSE
17     uytuyt pseudogibberish   FALSE
18    Semaiah            real    TRUE
19     iomnbm          random   FALSE
20    nqbthsh          random   FALSE
21      wwxnx          random   FALSE
22       bvgl          random   FALSE
23 Annabellee            real    TRUE
```

Text Featurization

```
fit <- rxFastLinear(
        is_real ~ chargrams,
        local_xdf,
        type="binary", normalize="no",
        l1Weight=0, l2Weight=1e-8,
        mlTransforms = featurizeText(
                vars = c(chargrams="name"),
                case='lower',
                keepNumbers=FALSE,
                keepDiacritics=FALSE,
                keepPunctuations=FALSE,
                charFeatureExtractor=ngramCount(
                        ngramLength=3,
                        weighting="tf",
                        maxNumTerms=1e8
                ),
                wordFeatureExtractor=NULL
        )
)
```

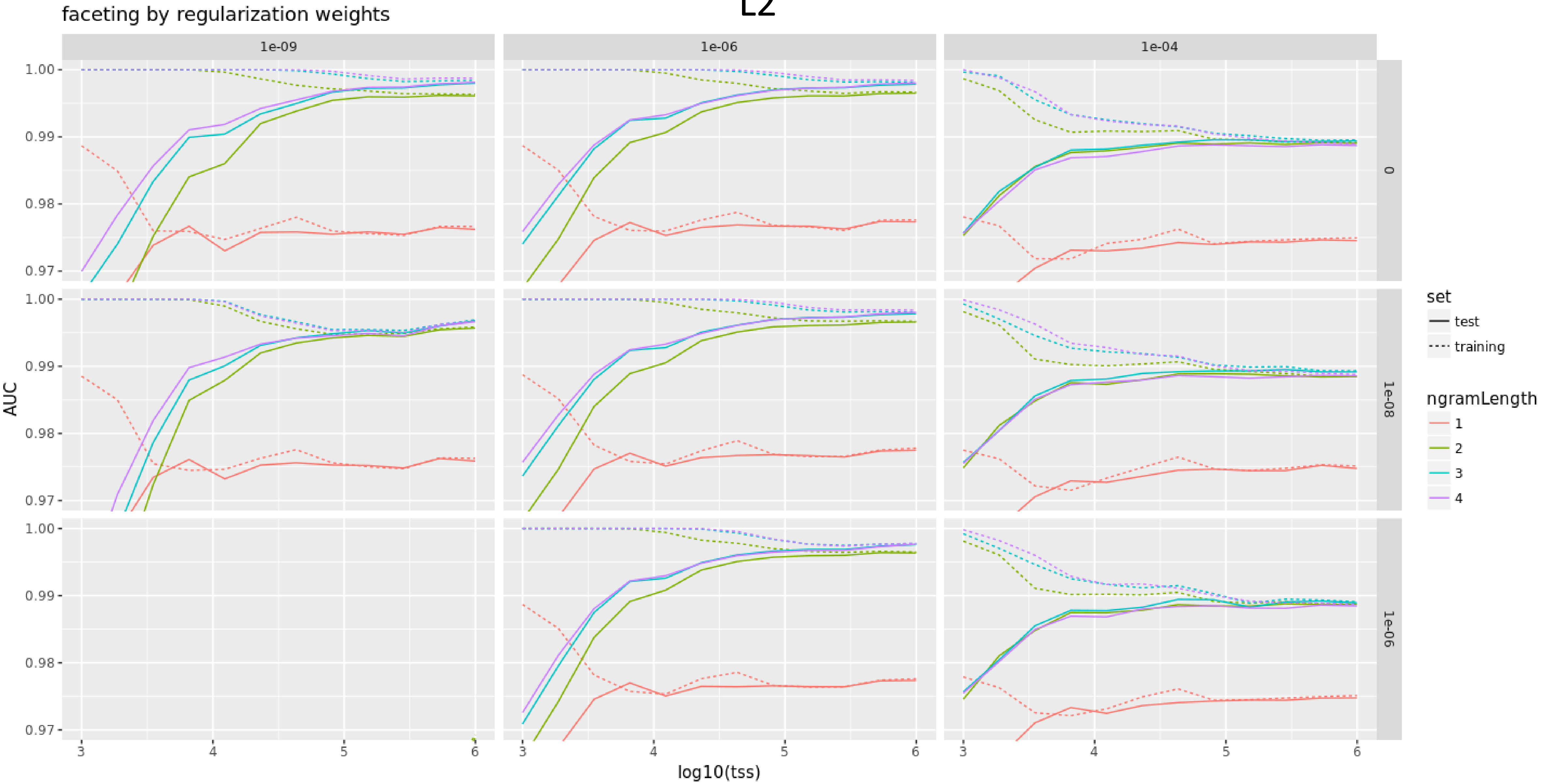
Model Coefficients

```
           coefficient
(Bias)     -10.71464
r|e|r      -17.37628
q          -15.18943
<⍰>|a|<⍰> -14.60359
q|u         13.91951
n|a|n      -13.82819
s|a|s      -13.79482
i|i        -13.73330
f|f         13.53813
<⍰>|l|u     13.33264
              ...
```

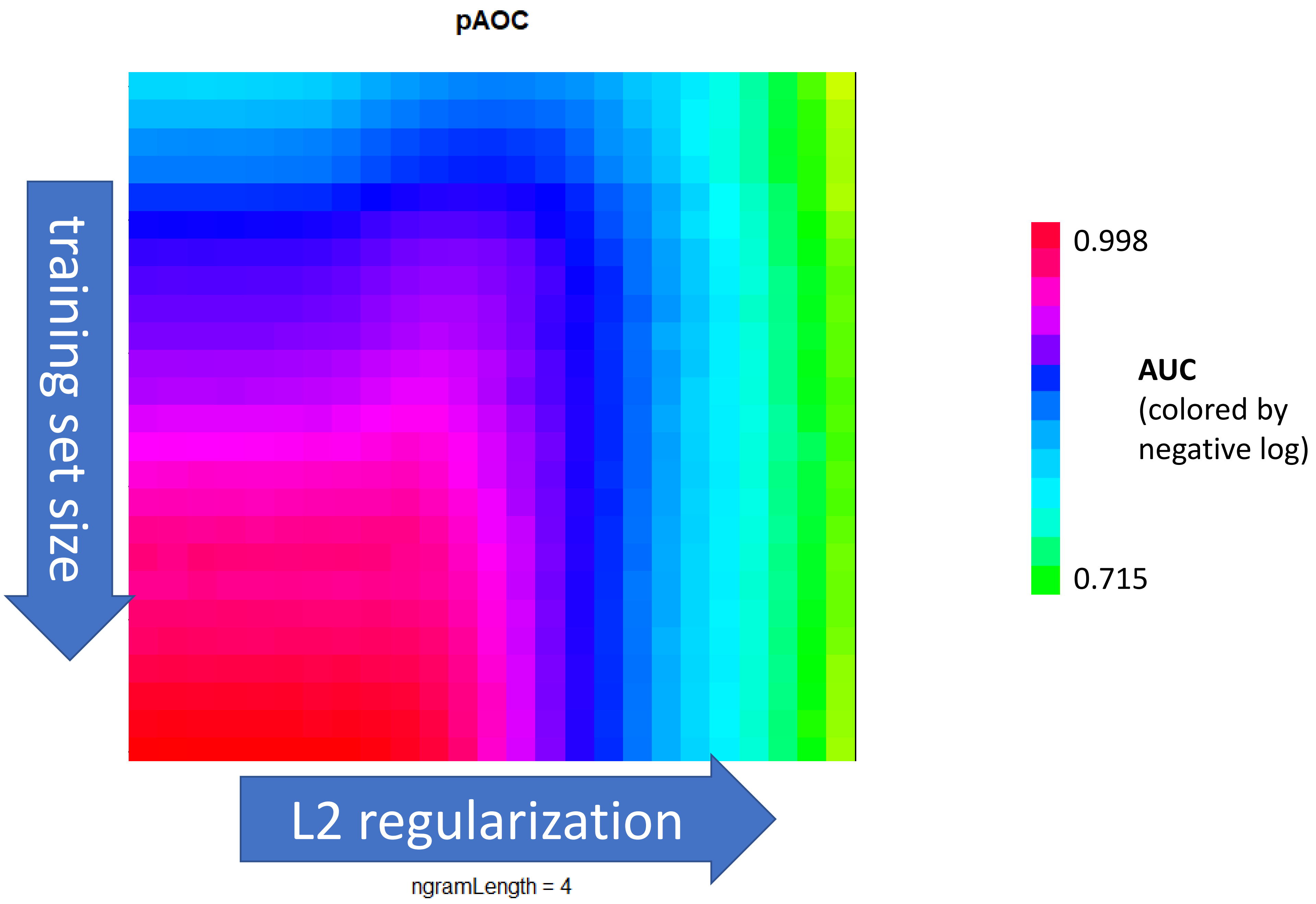
Tuning Regularization Penalties

L2

L1



Error Surface



training set size

L2 regularization

AUC
(colored by
negative log)

Grouped Time Series Forecasting

KDD 2017 – Using R for Scalable Data Science tutorial

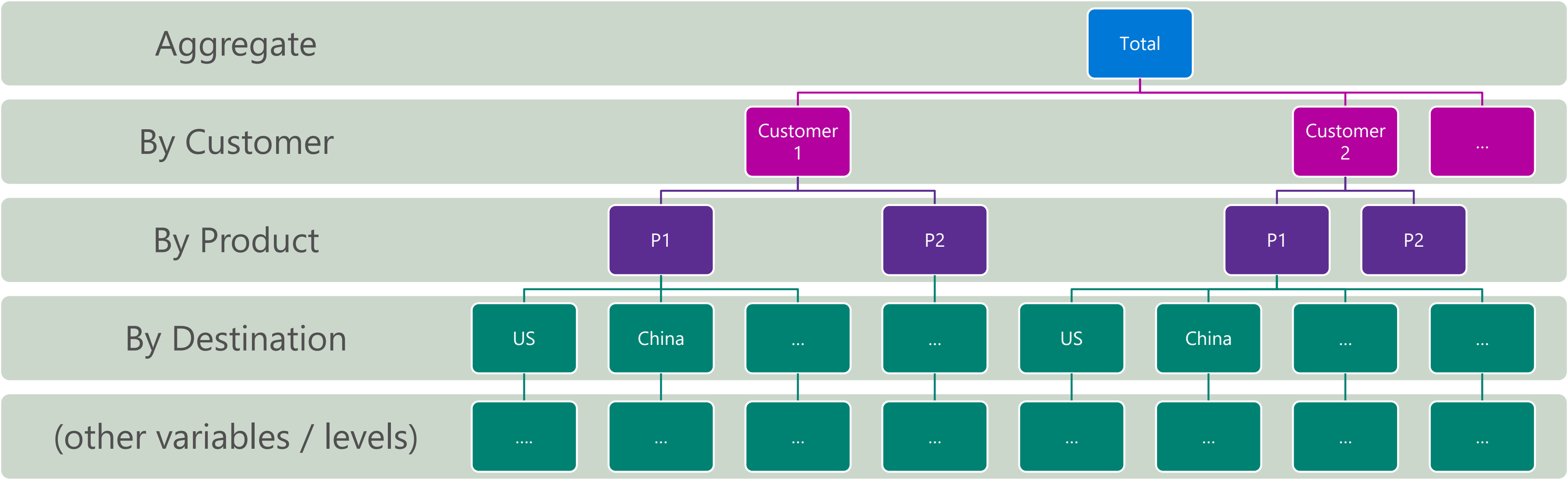
8/16/2017

Vanja Paunić
Data Scientist

Grouped Time Series (GTS) Forecasting

- Time series demand data can often be disaggregated by attributes of interest to form groups of time series or a hierarchy.

- For example, one might be interested in forecasting demand of all products in total, by location, by product category, by customer, etc.



Grouped time series forecasting | Concept

- Problem definition: use historical demand data to forecast demand in future periods across various **customers, products and destinations**.

- Forecasts need to be consistent across the groups / hierarchy
  - Lower level forecasts need to sum up to higher level forecasts

- We use **hierarchical (or more generally grouped) time series forecasting** to reconcile forecasts across the hierarchy

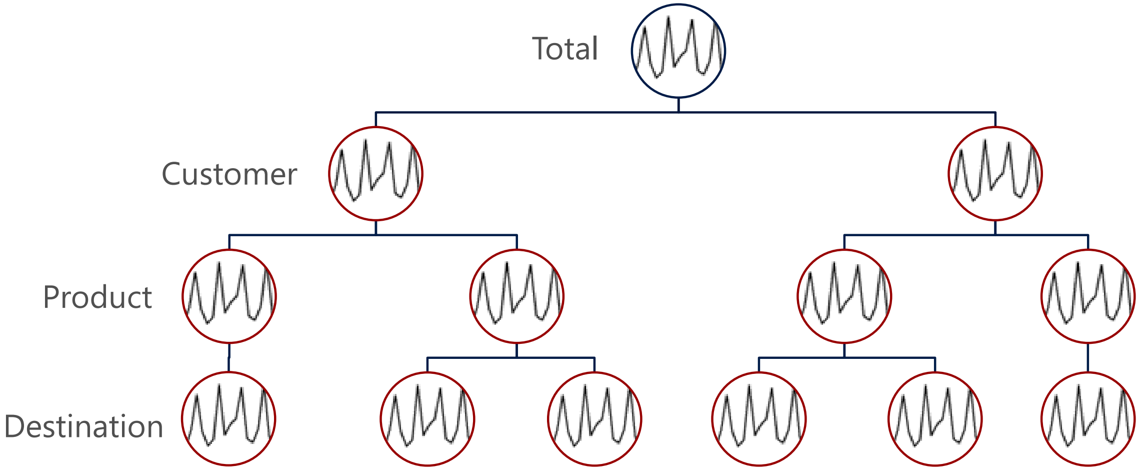
- Several approaches to GTS forecasting: bottom-up, top-down, middle-out

Grouped time series forecasting | Concept

Example Demand Data Set

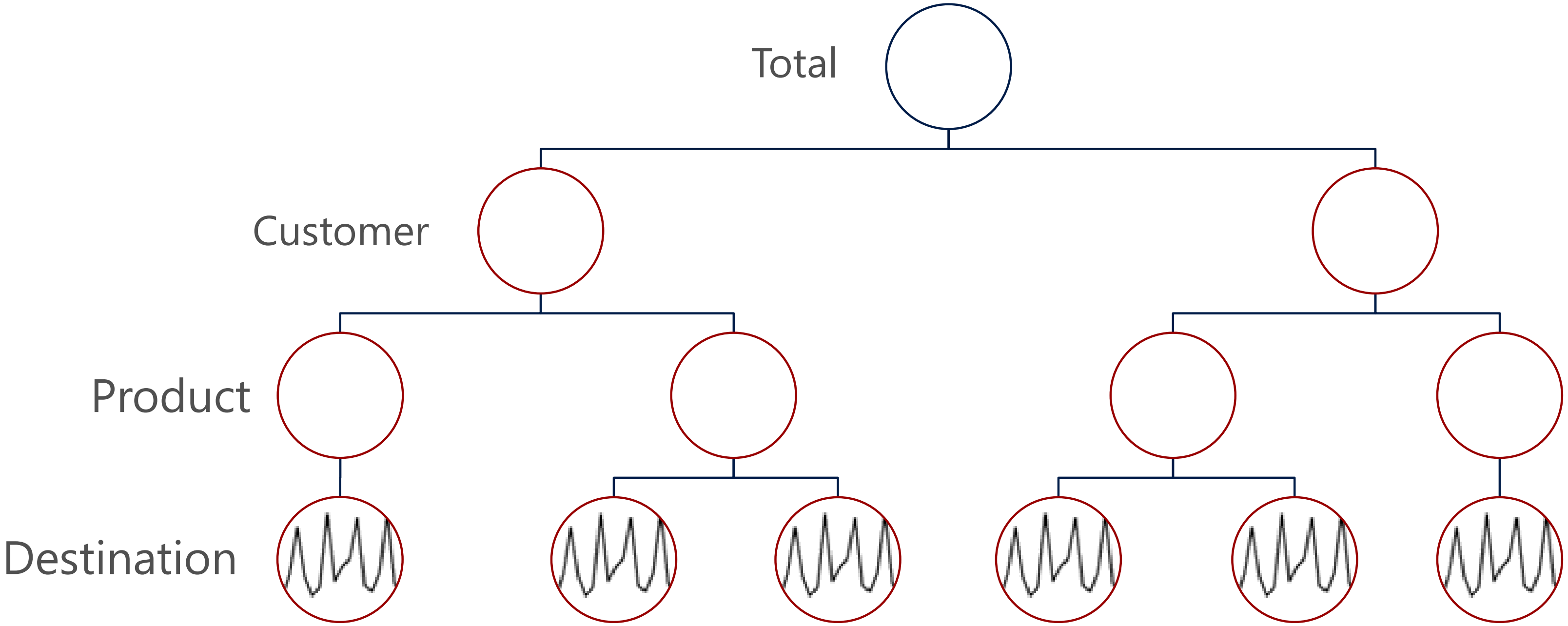
Customer	Product	Destination	Date	Quantity
Contoso	Metals	China	1/1/2015	84
Contoso	Metals	China	2/1/2015	80
Contoso	Metals	China	3/1/2015	97
Contoso	Metals	China	4/1/2015	85
Contoso	Metals	China	5/1/2015	97
Contoso	Metals	China	6/1/2015	93
Contoso	Metals	China	7/1/2015	91
Contoso	Metals	China	8/1/2015	87
Contoso	Metals	China	9/1/2015	93
Contoso	Metals	China	10/1/2015	94
Contoso	Metals	China	11/1/2015	82
Contoso	Metals	China	12/1/2015	74
Contoso	Metals	India	3/1/2015	47
Contoso	Metals	India	4/1/2015	39
Contoso	Metals	India	7/1/2015	41
Contoso	Metals	India	8/1/2015	44
Contoso	Metals	India	9/1/2015	51
Contoso	Metals	India	10/1/2015	61
Contoso	Metals	India	11/1/2015	66

Hierarchical or Grouped Time Series



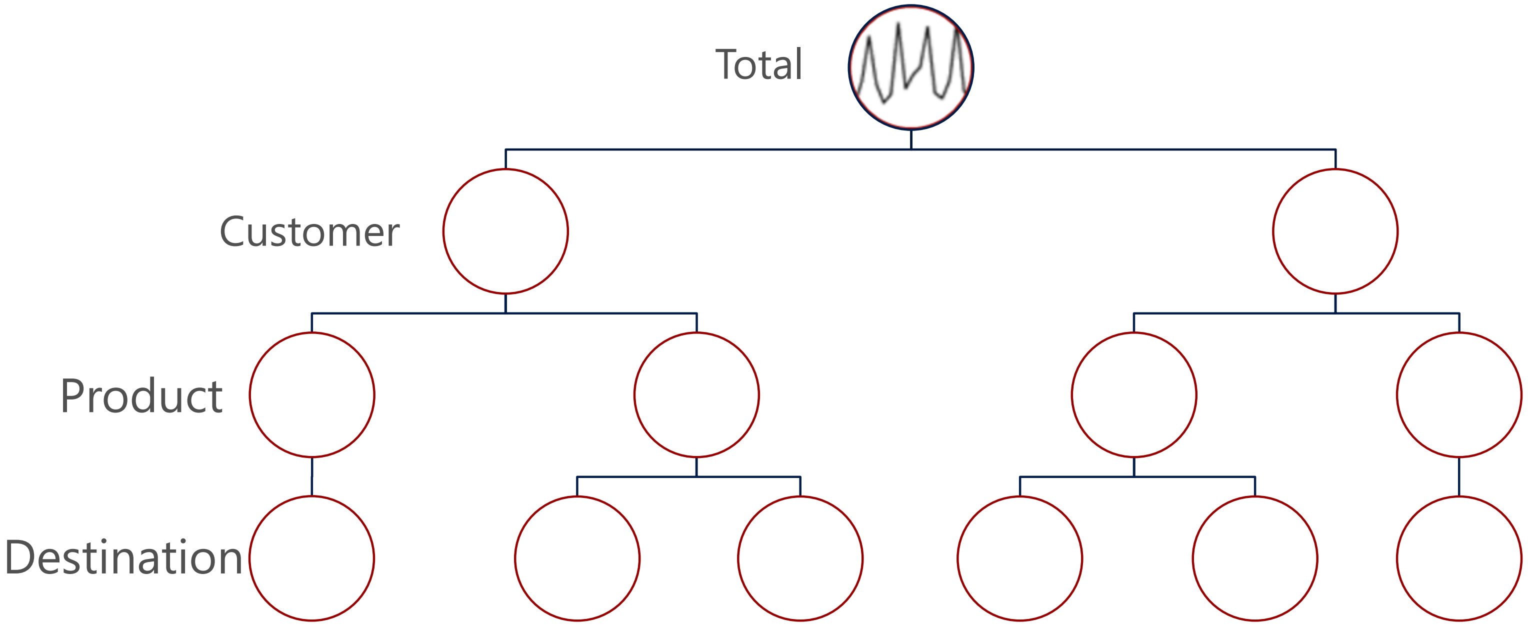
GTS Forecasting | Bottom-up Approach

- Forecast at lowest level, Destination, than use aggregation to obtain forecasts at levels above



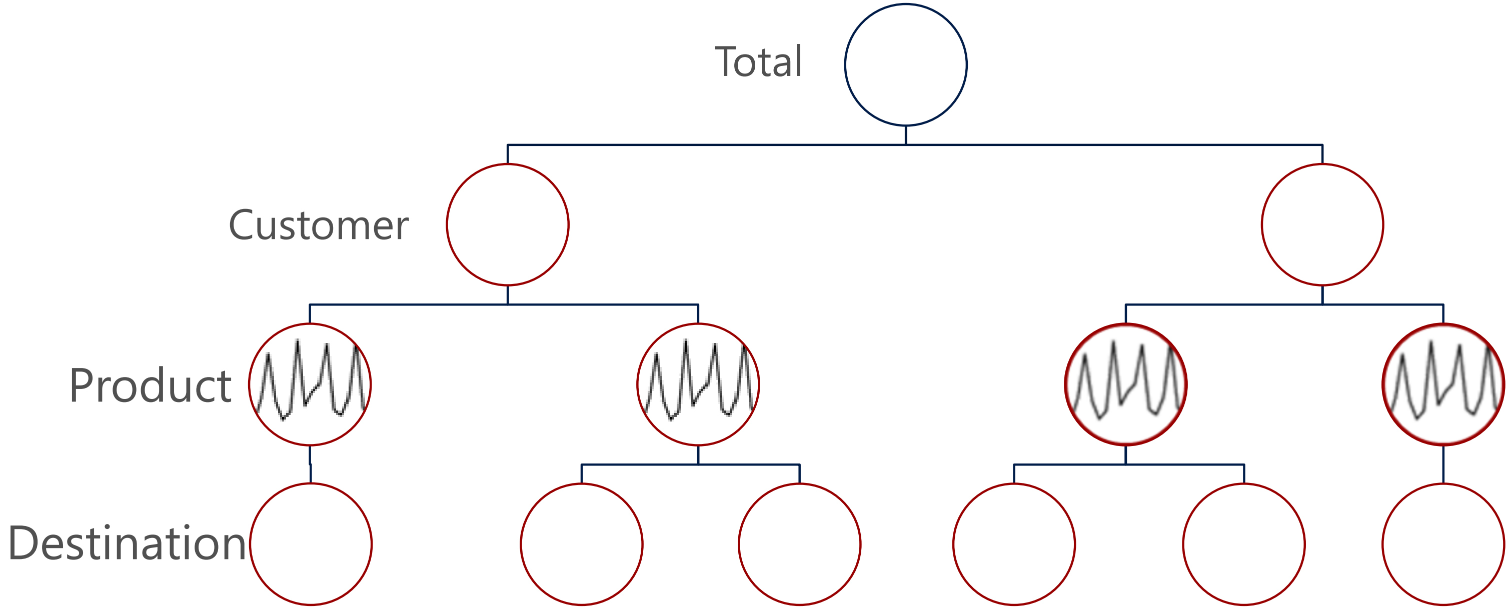
GTS Forecasting | Top-down Approach

- Forecast at the top level, Total, than use disaggregation based on historical proportions to obtain forecasts at lower levels.



GTS Forecasting | Middle-out Approach

- Forecast at some level, Level 2, than use aggregation to obtain forecasts at levels above, and disaggregation based on historical proportions to obtain forecasts at lower below.



Sentiment Analysis with Pretrained Deep Learning

Vanja Paunić
Data Scientist

Deep Learning in R

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Vanja Paunić
Data Scientist

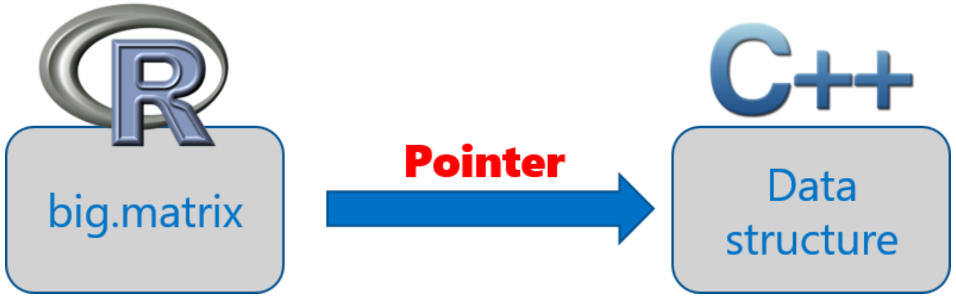
Package	Network Architecture	CPU / GPU support	Tensor backend	Reference
tensorflow TensorFlow for R	FFNN, CNN, RNN	CPU, GPU	Tensorflow	https://tensorflow.rstudio.com/
mxnet MXNet R API	FFNN, CNN, RNN	CPU, GPU	MXNet	http://mxnet.io/api/r/index.html
keras R interface for Keras	FFNN, CNN, RNN	CPU, GPU	Tensorflow, CNTK, Theano	https://rstudio.github.io/keras/
h2o - h2o.deepwater Deep Water R API	FFNN, CNN, RNN	CPU, GPU	Tensorflow, Caffe, MXNet	https://www.h2o.ai/deep-water/
h2o - h2o.deeplearning	FFNN	CPU	NA	http://docs.h2o.ai/h2o/latest-stable/h2o-docs/data-science/deep-learning.html
MicrosoftML Microsoft R Server	FFNN, CNN	CPU, GPU	NA	1) https://docs.microsoft.com/en-us/r-server/r-reference/microsoftml/rxneuralnet 2) https://blogs.msdn.microsoft.com/microsoftrservertigerteam/2017/03/10/get-started-with-microsoftmls-rxneuralnet-with-gpu-acceleration/

Other Options for Scaling R Scripts

Mario Inchiosa

The **`bigmemory`** project

- **`bigmemory`** supports large matrix-like objects in R
- Combines memory and file-backed data structures: analyze numerical data larger than RAM



- The data structures may be allocated to shared memory

Source: "The Bigmemory Project" by Michael Kane and John Emerson: April 29, 2010.

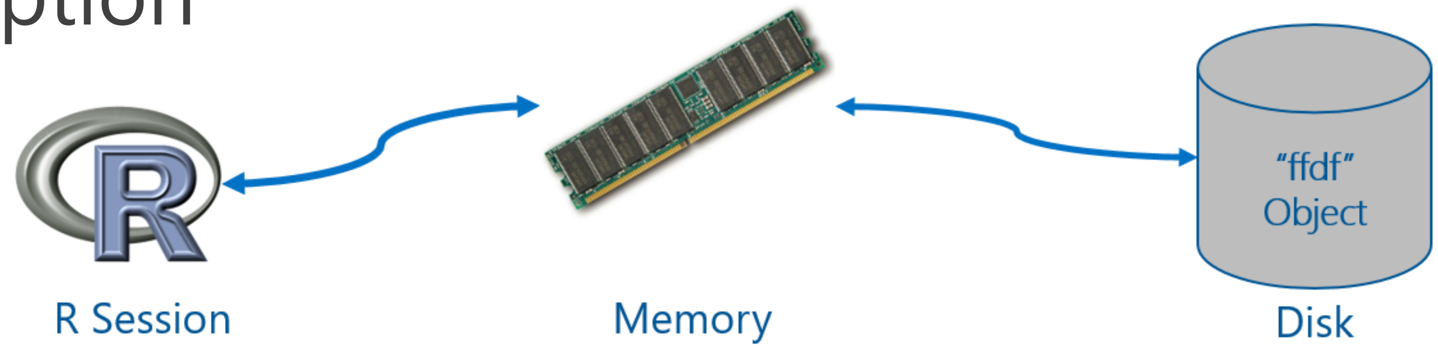
sister packages and related work

- **`biganalytics`**: provides exploratory data analysis functionality on big.matrix
- **`bigtabulate`**: adds table-, tapply-, and split-like behavior for big.matrix
- **`bigalgebra`**: performs linear algebra calculations on big.matrix and R matrix
- **`synchronicity`**: supports synchronization and may eventually support interprocess communication (ipc) and message passing
- **`biglm`**: provides linear and generalized linear models on big.matrix
- **`Rdsm`**: enables shared-memory parallelism with big.matrix

Source: "The Bigmemory Project" by Michael Kane and John Emerson: April 29, 2010.

`ff` package

- Provides data structures that are stored on Disk, but behave as if they were in RAM
- Maps only a section in main memory for effective consumption



- Accepts numeric and characters as input data

Source: ff: memory-efficient storage of large data on disk and fast access functions.

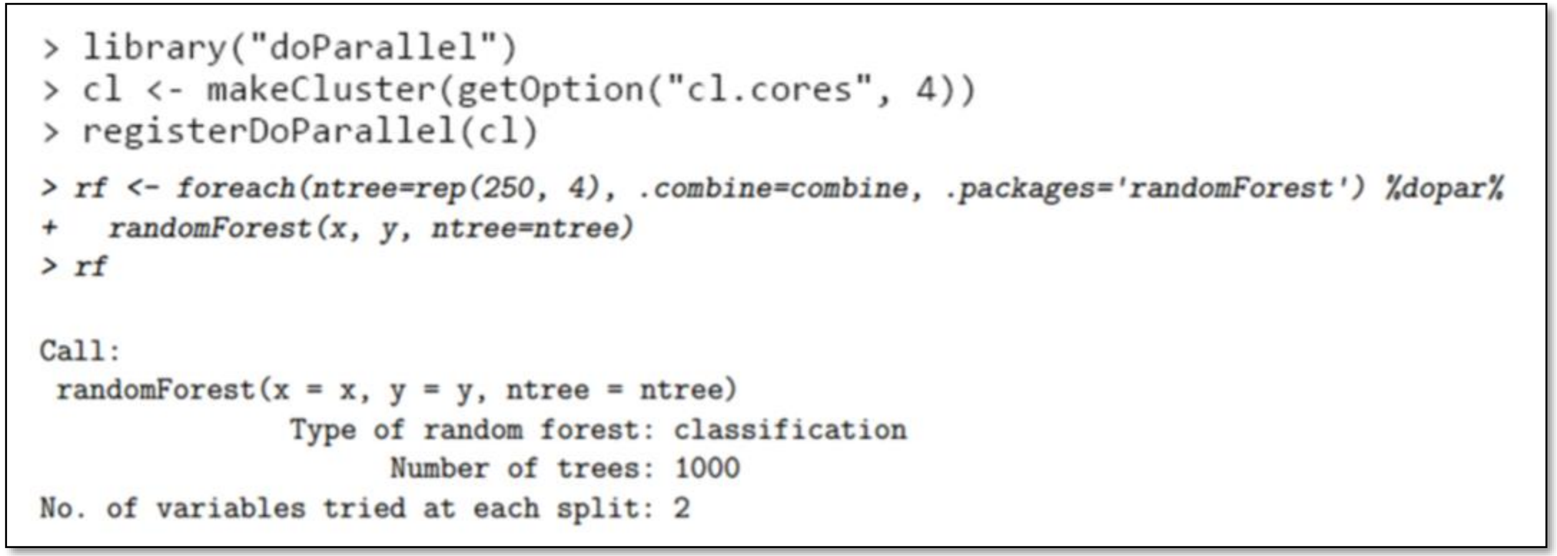
`ff` related packages

- **`ffbase`**: adds basic statistical functionality to ff
  - *Coercions*: as.character.ff(), as.Date_ff_vector(), as.ffdf.ffdf(), as.ram.ffdf()
  - *Selections*: subset.ffdf(), ffwhich(), transform.ffdf(), within.ffdf(), with.ffdf()
  - *Aggregations*: quantile.ff(), hist.ff(), sum.ff(), mean.ff(), range.ff(), tabulate.ff()
  - *Algorithms*: bigglm.ffdf()
- **`biglars`**: provides least-angle regression, lasso and stepwise regression on ff

Source: CRAN Task View: High-Performance and Parallel Computing with R, by Dirk Eddelbuettel.

Parallel programming with `foreach`

- Provides a function `foreach` and two operators `%do%` and `%dopar%` that support parallel execution
- `%dopar%` operator relies on a pre-registered parallel backend – `doParallel()`, `doSNOW()`, `doAzureParallel()`, etc.



```
> library("doParallel")
> cl <- makeCluster(getOption("cl.cores", 4))
> registerDoParallel(cl)
> rf <- foreach(ntree=rep(250, 4), .combine=combine, .packages='randomForest') %dopar%
+   randomForest(x, y, ntree=ntree)
> rf

Call:
 randomForest(x = x, y = y, ntree = ntree)
               Type of random forest: classification
                     Number of trees: 1000
No. of variables tried at each split: 2
```

Source: foreach package.

Q & A

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THANK YOU