## Data Science

joaquin vanschoren


WHAT IS DATA SCIENCE?

## Hacking skills

## Expertise

Maths \& Stats





## THE HYPE



## THE HYPE

"Data Scientist: The Sexiest Job of the 21 st Century"

- Harvard Business Review
"Whenever you read about data science or data analysis, it's about the ability to store petabytes of data, retrieve that data in nanoseconds, then turn it into a rainbow with a unicorn dancing on it."
- David Coallier


## THE REALITY



- You'll clean a lot of data. A LOT
- A lot of mathematics. Get over it
- Some days will be long. Get more coffee
- Not everything is about Big Data
- Most people don't care about data
- Spend time finding the right questions

Big Data and Open Data are fun, but what really matters is what you learn from it.

## Data Scientific Method



Based on an observation


Create an Hypothesis


FEATURES,


Test Hypothesis


Won't be pretty, repeat

LET DATA FRAME THE CONVERSATION

Data gives you the what Humans give you the why

## CONVERSE

- What data is missing? Where can we get it?
- Automate data collection
- Clean data, then clean it more
- Visualize data: the brain sees
- Merge various sources of information
- Reformulate hypotheses
- Reformulate questions



## DATA SCIENCE TOOLS



Matt Turck (@mattturck) and ShivonZilis (@shivonz) Bloomberg Ventures
modelling, testing, prototyping
lubridate, zoo: dates, time series reshape2: reshape data ggplot2: visualize data RCurl, RJSONIO: find more data HMisc: miscellaneous DMwR, mlr: machine learning Forecast: time series forecasting garch: time series modelling quantmod: statistical financial trading xts: extensible time series igraph: study networks maptools: read and view maps

scientific computing
numpy: linear algebra
scipy: optimization, signal/image processing, ...
scikits: toolkits for scipy
scikit-learn: machine learning toolkit statsmodels: advanced statistic modelling matplotlib: plotting
NLTK: natural language processing PyBrain: more machine learning PyMC: Bayesian inference Pattern:Web mining NetworkX: Study networks Pandas: easy-to-use data structures


(3) RAPID|MINER

KNIMIE

## MapReduce


shuffle

worker nodes (local)
worker nodes (local)
$\xrightarrow{\text { mapper }}$ node

remote
read

## $\xrightarrow[\text { node }]{\text { reducer }}$








## Mapper <br> Reducer



# Input Intermediate file file (local) 

Output file
<a,apple> <a',slices>

Input file


Intermediate file
<a',slices>

<p,pineapple>

Output file

<a,apple>

shuffle

worker nodes (local)
worker nodes (local)
shuffle + parallel sort

Google chicken is a

## Google

## Map phase (3 parallel tasks)

- $\operatorname{map}_{1}=>\left(\right.$ "why", $\left.\left(d o c_{1}, 1\right)\right)$, ("did",(doc $\left.{ }_{1}, 2\right)$ ), ("the", $\left(d o c_{1}, 3\right)$ ),
("chicken", (doc $\left.{ }_{1}, 4\right)$ ), ("cross",( doc $\left._{1}, 5\right)$ ), ("the", $\left(d o c_{1}, 6\right)$ ),
("road",(doc ${ }_{1}$, 7))
- $\operatorname{map}_{2}=>\left(" t h e^{\prime \prime},\left(\right.\right.$ doc $\left.\left._{2}, 1\right)\right)$, ("chicken",(doc 2,2$\left.)\right)$, ("and", $\left(\right.$ doc $\left._{2}, 3\right)$ ),
("egg",(doc 2,4$)$ ), ("problem", (doc $\left.{ }_{2}, 5\right)$ )
$-\operatorname{map}_{3}=>\left(" k e n t u c k y\right.$ ", $\left(\right.$ doc $\left._{3}, 1\right)$ ), ("fried", $\left(\right.$ doc $\left._{3}, 2\right)$ ), ("chicken", $\left(d o c_{3}, 3\right)$ )

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## Google

```
Intermediate shuffle \& sort phase
    - ("why", <(doc \(\left.{ }_{1}, 1\right)>\) ),
    - ("did", <(doc \(\left.{ }_{1}, 2\right)>\) ),
    - ("the", <(doc \(\left.\left.{ }_{1}, 3\right),\left(d o c_{1}, 6\right),\left(d o c_{2}, 1\right)>\right)\)
    - ("chicken", <(doc 1,4\(\left.),\left(d o c_{2}, 2\right),\left(d o c_{3}, 3\right)>\right)\)
    - ("cross", <(doc \(\left.{ }_{1}, 5\right)>\) )
    - ("road", <(doc \(\left.{ }_{1}, 7\right)>\) )
    - ("and", <(doc 2,3\()>\) )
    - ("egg", <(doc \(\left.{ }_{2}, 4\right)>\) )
    - ("problem", <(doc 2,5\()>\) )
    - ("kentucky", <(doc \({ }_{3}\), 1)>)
    - ("fried", <(doc \(\left.{ }_{3}, 2\right)>\) )
```

```
Reduce phase (11 parallel tasks)
    - ("why", <(doc \(\left.{ }_{1},<1>\right)>\) ),
    - ("did", <(doc \(\left.{ }_{1},<2>\right)>\) ),
    - ("the", <(doc \(\left.{ }_{1},<3,6>\right),\left(\right.\) doc \(\left.\left._{2},<1>\right)>\right)\)
    - ("chicken", <(doc \(\left.1,<4>),\left(d o c_{2},<2>\right),\left(d o c_{3},<3>\right)>\right)\)
    - ("cross", <(doc \(\left.{ }_{1},<5>\right)>\) )
    - ("road", <(doc \(\left.{ }_{1},<7>\right)>\) )
    - ("and", <(doc \(\left.{ }_{2},<3>\right)>\) )
    - ("egg", <(doc \(\left.{ }_{2},<4>\right)>\) )
    - ("problem", <(doc \(\left.2_{2},<5>\right)>\) )
    - ("kentucky", <(doc \(\left.{ }_{3},<1>\right)>\) )
    - ("fried", <(doc \(\left.{ }_{3},<2>\right)>\) )
```


## Nearest bar

## Input

graph
(node,label)


## Nearest bar

## Input

graph (node,label)

Map
$\forall$, search graph with radius $d$ < , \{0 , distance\} >


## Nearest bar

Input
graph (node,label)

Map
$\forall$, search graph
<, , 0 , distance $\}$ by id


## Nearest bar

Input
graph (node,label)

Map
$\forall$, search graph
< , \{0, distance\} > by id

Shuffle/ Reduce
< , , $\{$, , distance\}, \{0, distance\}] >
-> min()


Output

marked graph


## EXAMPLES




Strain (transverse)
$00: 00: 00$

$$
\begin{gathered}
g * h \equiv \int_{-\infty}^{\infty} g(\tau) h(t-\tau) d \tau \\
(r * s)_{j} \equiv \sum_{k=-M / 2+1}^{M / 2} s_{j-k} r_{k}
\end{gathered}
$$

## convolution

# MATHS 

Convolution


## COMPLEXITY



## SCALE-SPACE



# SCALE-SPACE DECOMPOSITION 



# | 45 sensors <br> 100 Hz <br> 5GB/day <br> 2TB/year <br> 50MB/s disk I/O 



VOLUME
MapReduce
data: 2008-10-24 06:15:04.559, -6.293695, -1.1263204, 2.985364, 43449.957, 2.3577218, 38271.21 question: min, mean, max signal over all strain sensors?
public void map(LongWritable key, Text value, Context context) \{
String values[] = value.toString().split("lt");
Text time = new $\operatorname{Text}($ values[0]);
for(int $\mathrm{i}=1$; $\mathrm{i}<=$ nrStressSensors; $\mathrm{i}++$ )
context.write(time, new Text(values[i]));
\}
public void reduce(Text key, Iterable<Text> values, Context context) \{
//init; sum, min, max, count = 0
Double d;
for (Text v : values) \{
$\mathrm{d}=$ Double.valueOf(v.toString());
sum += d;
$\min =$ Math. $\min (\min , d)$;
$\max =$ Math. $\max (\max , \mathrm{d})$;
count++;
\}
context.write(new Text(key+" min"), new Text(Double.toString((min)))); context.write(new Text(key+" max"), new Text(Double.toString((max)))); context.write(new Text(key+" avg"), new Text(Double.toString((sum/count))));

## CONVOLUTION




Emit only unpolluted data


Map
(convolute
with 0 -padding)
Reduce (add)

0


0
0
0

Add values in overlapping regions

CONVOLUTE-ADD

## SEGMENTATION

- You don't need 100 Hz data for everything
- Approximate signal with linear segments
- Key points: 0-crossings of Ist, 2nd, 3rd derivative
- Maths: derivative of smoothed signal = convolution with derivative of kernel
signal
convolution segmentation


## Ist, 2nd,3rd degree derivatives

## SEGMENTATION RESULT




## TRACKING NEWS STORIES

But Will It Make You Happy?
By STEPHANIE ROSENBLOOM
Mon Aug 09 10.46:09 EDT 2010



## Geospacial data

## 6AM <br> New York City

Arts \& Entertainment

College \& University

Nightlife Spot 8

## $\square$

Great Outdoors

Shop \& Service

Professional \& Other Places
Travel \& Transport

## Residence

## Food

Travel \& Transport
8

## foursquare <br> Ce

(Tc)
 K라 CALM AND
ANALYZE B|G DATA

## OPEN DATA OPEN SCIENCE

## THE OPEN DATA MOVEMENT

## THE EVOLUTION OF APIs

Increasingy, companies are making their data and inner workings publicly avalable through the release of APIs, which are used by developers in buldng now tools- Mie TweetDock, basod on Twatters APL. Since 2005, more than 3,700 APIs have been launched.

## WHAT IS AN API?

An application programming interface is a set of instructions that allows software programs to interact wth each other. ProgrammableWes tracks AP1s and "mashups" (new combinations of existing AP1s).

300 4,000
NEW APIs TOTAL APIs by month cumulative

## PUBLLC DATA AROUND THE WORLD

From education to energy, heath to poverty, and finance fo
dernographics, governments and NGOs are opening up their data dernographics, governments and NGOS are opening up their data
troves sa, that aryone can look for patterns and create informed
solutions to global chalenges.

Fingal County led the way in opening its data, which wre used at the coungr's frst open data chatenge in thty 2011. Duttin City will open in Septerrber 2011.

## Ireland



Data.gov.uk contains more than 7,200 datasets from seven govermmental pubishers, including 989 from the Department of Health and 784 from the Dupartment for Commurites and loca



## 1609

GALILEO GALILEI DISCOVERS SATURN'S RINGS

WHAT DID HE DO?

## 1450

## PRINTING PRESS

## 1609

GALILEO GALILEI ANAGRAMS

## 1 8TH CENTURY

 SCIENTIFIC REVOLUTIONJOURNAL ACCEPTED AS BEST WAY TO ADVANCE SCIENCE

Are journals still the best we can do?
We have the internet, but publish results on paper?

## openml.org

An open science platform for machine learning


Search 575889 experiments on 130 datasets and 191 algorithm/workflow implementations

## openml.org

## Share results <br> Search results



Integrated in machine learning tools

## Search: Free text

| Q All | OpenML | Search | Share | Plugins | Developers | Community | 2 Sign in |  | $y$ in $8^{+}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 曲 Datasets | (tisplemen | tions | .all Metrics | Tasks | 4 Runs | $\triangle$ Advanced | SQL | @ Graph | Results |
| Search |  |  |  |  |  |  |  |  |  |  |
| tree |  |  |  |  |  |  |  |  | Q |  |

Found 40 results ( 0.083 seconds)

* weka.J48(1.2)

Implementation for generating a pruned or unpruned C4.5 decision tree. For more information, see Ross Quinlan (1993). "C4.5: Programs for Machine...
77404 runs
© molecular-biology_promoters

1. Title of Database: E. coli promoter gene sequences (DNA) with associated imperfect domain theory 2 . Sources: (a)... 6264 runs
ⓘc-tac-toe
2. Title: Tic-Tac-Toe Endgame database 2. Source Information -- Creator: David W. Aha (aha@cs.jhu.edu) -- Donor: David W. Aha...

5356 runs
bridges_version2

1. Title: Pittsburgh bridges 2. Sources: -- Yoram Reich \& Steven J. Fenves Department of Civil Engineering and ... 5203 runs

## Search: Algorithm detail

## weka.J48(1.2)

## Beta

(3) General Information

Runs

롤 Algorithm Parameters

Algorithm Properties

Use the dropdown below to select which evluation measure should be used.


## Search: Run detail

## weka.J48(1.2)

## Beta

(5) General Information

* Runs

롤 Algorithm Parameters

Algorithm Properties

Use the dropdown below to select which evluation measure should be used.


## Search: Algorithm parameters

## weka.J48(1.2)

## Beta

(i) General Information
$\star$ Runs

롤 Algorithm Parameters

- Algorithm Properties

| 50 * | records per page |  | Showing 1 to 10 of 10 entries |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Name ${ }^{\text {A }}$ | General Name | Description | Data Type | Default <br> Value | Minimum | Maximum |
| A | used lapace smoothing for predicted probabilities |  | enum(true,false) | false |  |  |
| B | use binary splits for nominal attributes |  | enum(true,false) | false |  |  |
| C | confidence threshold for pruning | default 0.25 | double | 0.25 | 0.01 | 0.99 |
| L | switch off cleaning up after tree has been built |  | enum(false) | todo |  |  |
| M | minimum nb instances per leaf | default 2 | $\operatorname{int}(11)$ | 2 | 2 | 20 |
| N | nb folds for reduced error pruning | one fold is used as pruning set | int(11) | 3 | 2 | 10 |

## Search: Algorithm properties

## weka.J48(1.2)

## Beta

## (3) General

 InformationRuns

롤 Algorithm Parameters

D Algorithm Properties

$50 \quad$ records per page
$\left.\begin{array}{|l|l|l|}\hline \text { Name } & \text { Description } & \text { Value } \\ \hline \text { BiasVarianceProfile } & \begin{array}{l}\text { The weight of the bias component in the learning algorithm's } \\ \text { error. I.e., the percentage of errors that can be attributed to bias } \\ \text { error (underfitting) as opposed to variance error (overfitting). }\end{array} & 0.67804121865815 \\ \hline \text { BiasWeightKohaviWolpert } & \begin{array}{l}\text { empirically calculated average ratio of bias error in the total } \\ \text { error, using Kohavi-Wolpert's definition of bias and variance }\end{array} & 0.67804121865815 \\ \hline \text { BiasWeightWebb } & \text { empirically determined average ratio of bias error in the total } \\ \text { error, using Webb's definition of bias and variance }\end{array}\right) 0.772941309061007$.

## Search: Dataset detail

OpenML Search Share Plugins Developers Community a Sign in in

## (3) General

 Information* Runs
- Data Features
\$ Data Properties

By default only the results of the best parameter settings are shown. Press the "Show all/best results" button to include all results. Use the dropdown below to select which evaluation measure should be used.


## Search: Dataset properties

Beta

## (1) General

## Information

Runs

- Data Features

Data Properties
$50 \quad$ records per page

| Name | Description | Value |
| :--- | :--- | :--- | :--- |
| DefaultAccuracy | The predictive accuracy obtained by simply predicting the <br> majority class. | 0.333333 |
| EntropyClass | Entropy of the class attribute. It determines the amount of <br> information needed to specify the class of an instance, or <br> how 'informative' the attributes need to be. A low class <br> entropy means that the distribution of examples among <br> classes is very skewed (containing some very infrequent <br> classes) which some algorithms cannot handle well. | 1.58496 |
| FeatureAbsoluteSkewness | Absolute skewness values over all features. Usually, the <br> min,max and mean are calculated. Skewness is a measure of <br> how non-normal a feature's value distribution is. Many <br> learning algorithms assume normality. | 0.339639 |
| FeatureAbsoluteSkewness | Absolute skewness values over all features. Usually, the <br> min,max and mean are calculated. Skewness is a measure of <br> how non-normal a feature's value distribution is. Many | 0.0189027 |

## Search: Quick comparisons



A comma separated list of implementations. Leave empty to include all al gorithms.

## Datasets

Collection:uci,
A comma separated list of datasets. Leave empty to include all datasets.

Iミ Advanced options

## Search: Quick comparisons



## Search: Visualizations

OpenML


## Open Controls

圆

IE Table
(1ill Scatterplot
(hll) Line plot

name
$\rightarrow$ weka.J48(1.2) -- weka.SMO(1.53.2.2)

## Search: Advanced queries



## Advanced queries

Click a query to run it, or edit the query in the SQL tab.

## Comparison

Comparing all algorithms in the database on a specific dataset D

Directly compare two algorithms on all datasets

Comparing all algorithms in the database, on a specific dataset $D$, and distinguish between baselearners used in ensembles and kernels used in kernel methods

Compare all algorithms (including different base-learners and kernels) over all UCI datasets, using a range of evaluation metrics, all normalized between the baseline (default accuracy) and maximum performance.

Show the best algorithm per dataset, and its predictive accuracy

## Data Properties

Show the effect of data property DP on the optimal value of parameter $P$

Show the performance difference of two algorithms, ordering datasets by time of publication

## Search: Parameter effects

## OpenML Search Share Plugins Developers Community a Sign in


(1ill) Scatterplot
(1.1) Line plot


## Search: Parameter effects



Datasets in order of increasing size

## Search: Learning curves



## Meta-models




## @joavanschoren

