Data Science joaquin vanschoren



WHAT IS DATA SCIENCE?

Hacking skills

Expertise

Maths & Stats

Hacking skills

Danger zone! Machine Learning Data Science

Expertise

Research

Maths & Stats

[Drew Conway]

(data) science officer



[Joel Grus]



THE HYPE



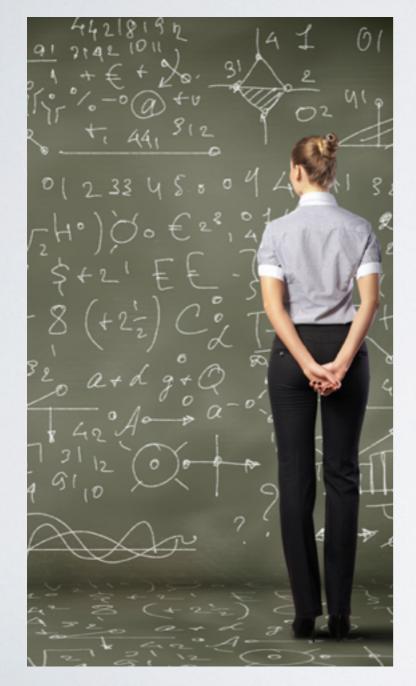
THE HYPE

"Data Scientist: The Sexiest Job of the 21st 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

[David Coallier]

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

Data Scientific Method



SIAR AOUESTION

Based on an observation

ANAI YSE **()**RRFNT |A|A

Create an Hypothesis

(RHAIF FEATURES, EXPERIMENT

Test Hypothesis

ANALYSE RESULTS

Won't be pretty, repeat

LEIDATA FRAME IHF 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

PYTHON 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

OTHER

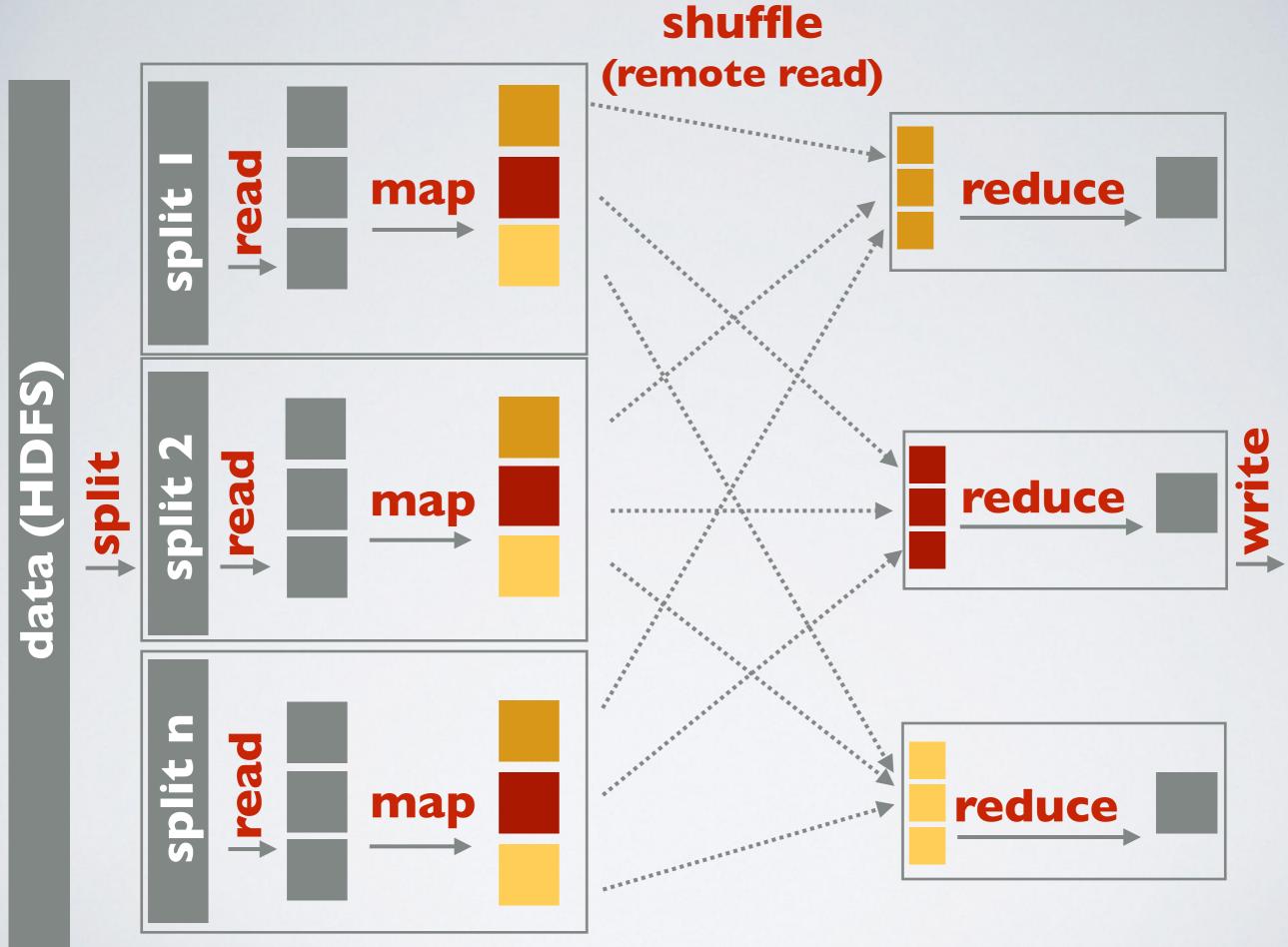








<u>Maprecues</u>

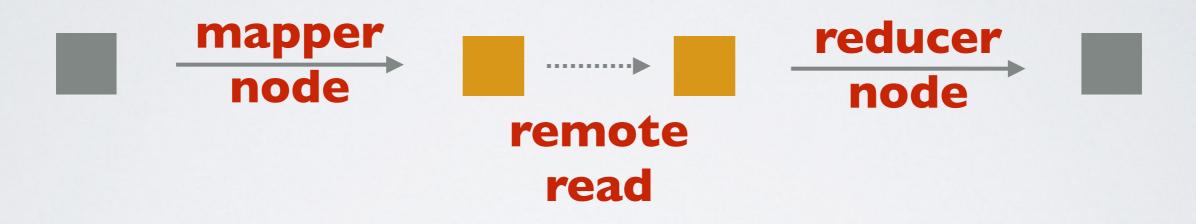


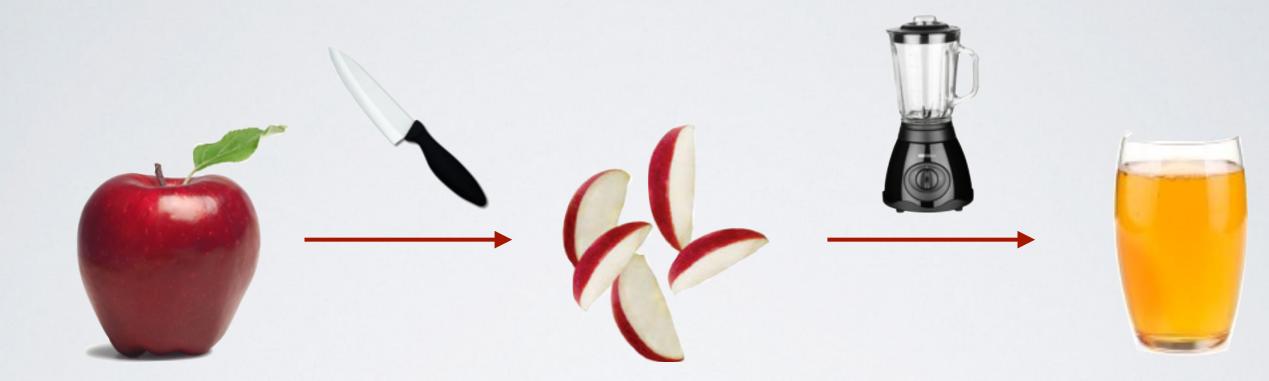
worker nodes (local)

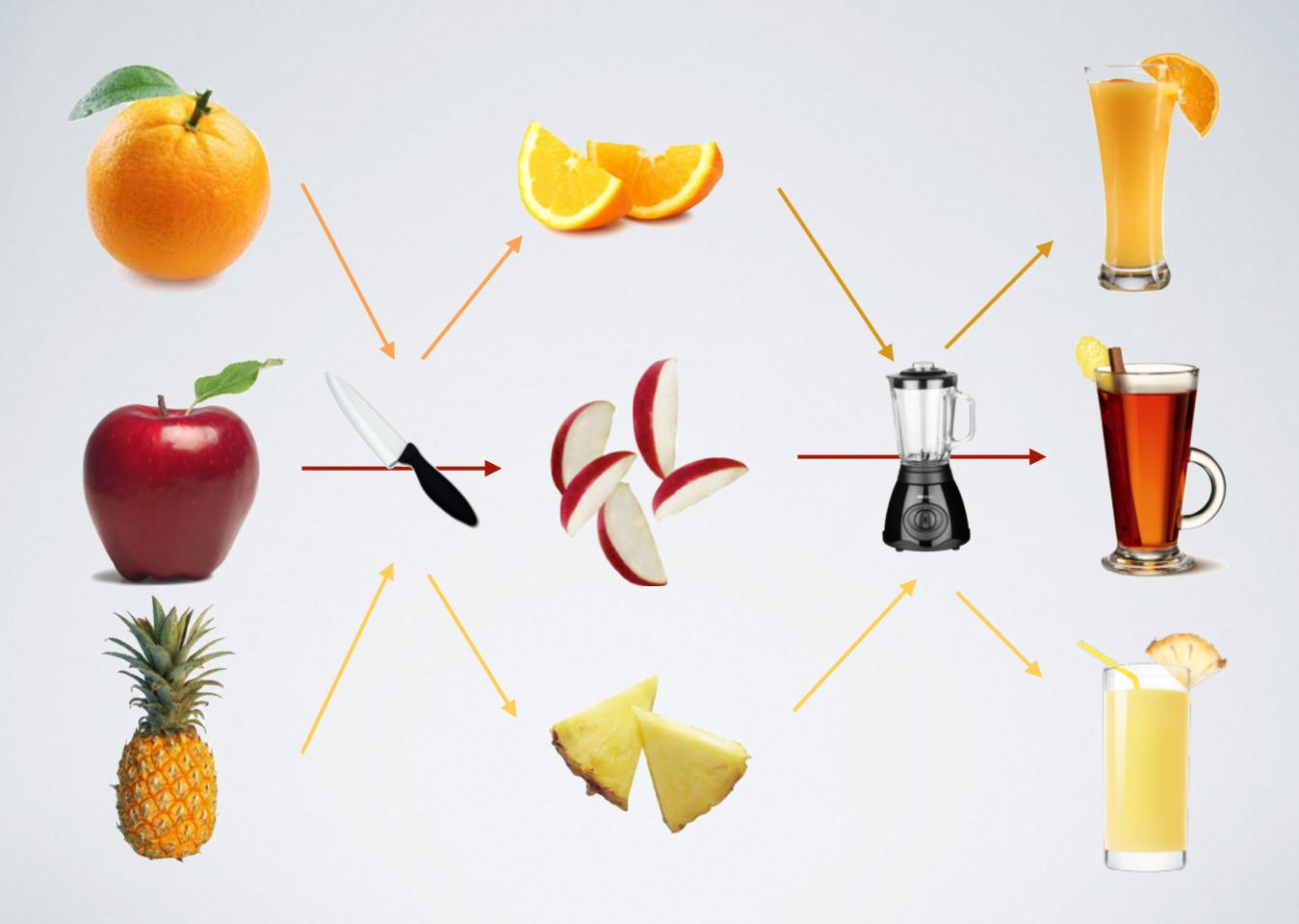
worker nodes (local)

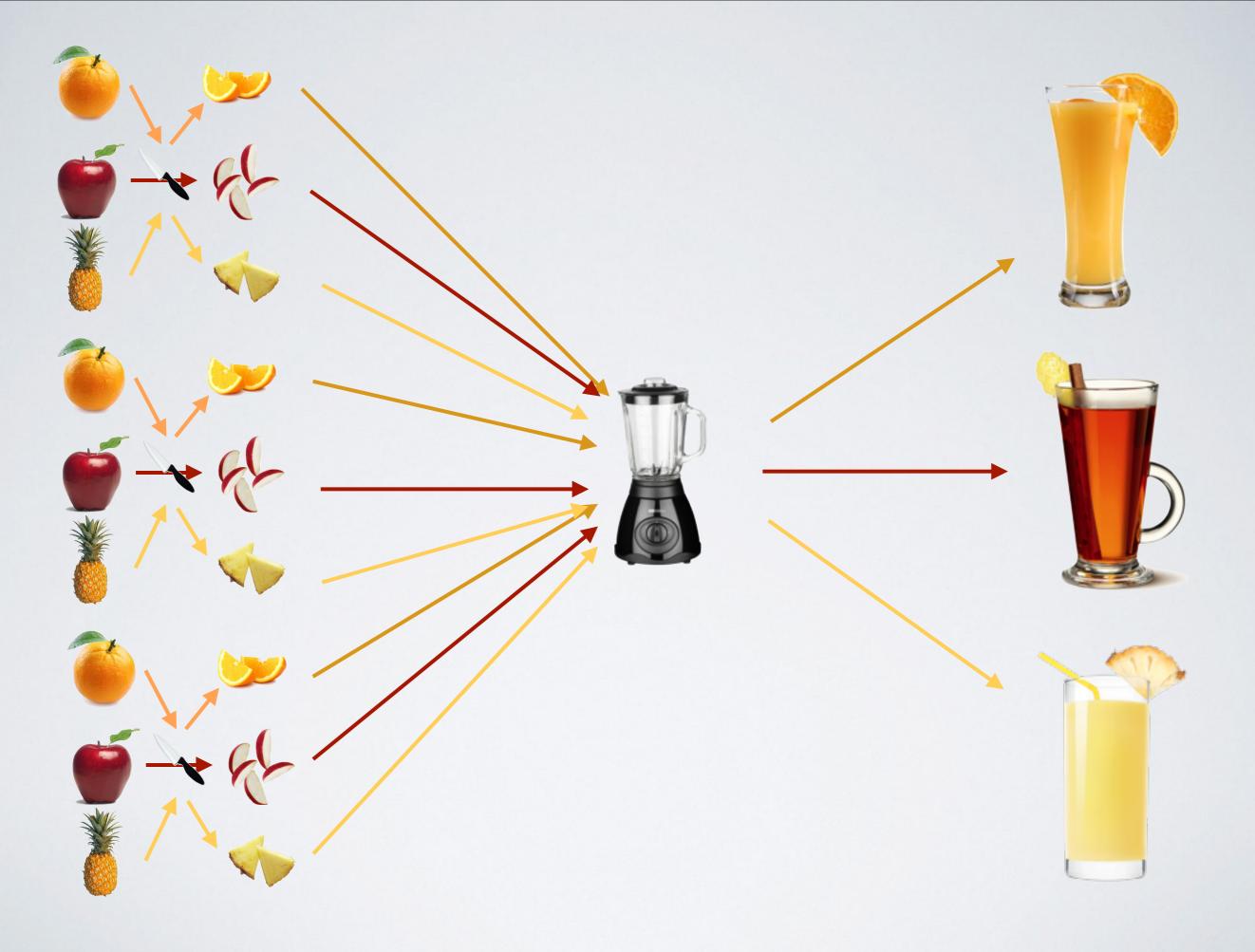
(HDFS)

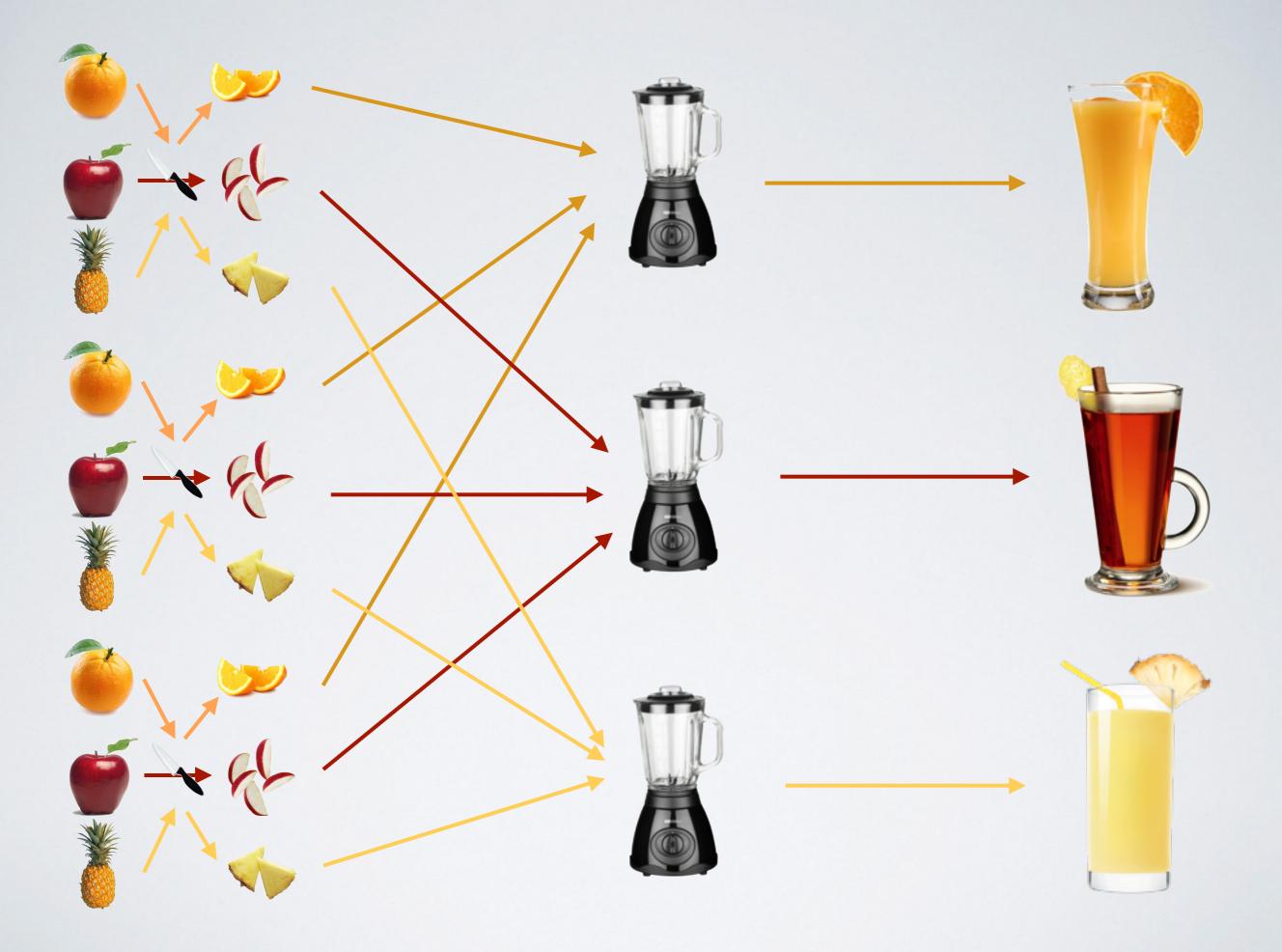
data

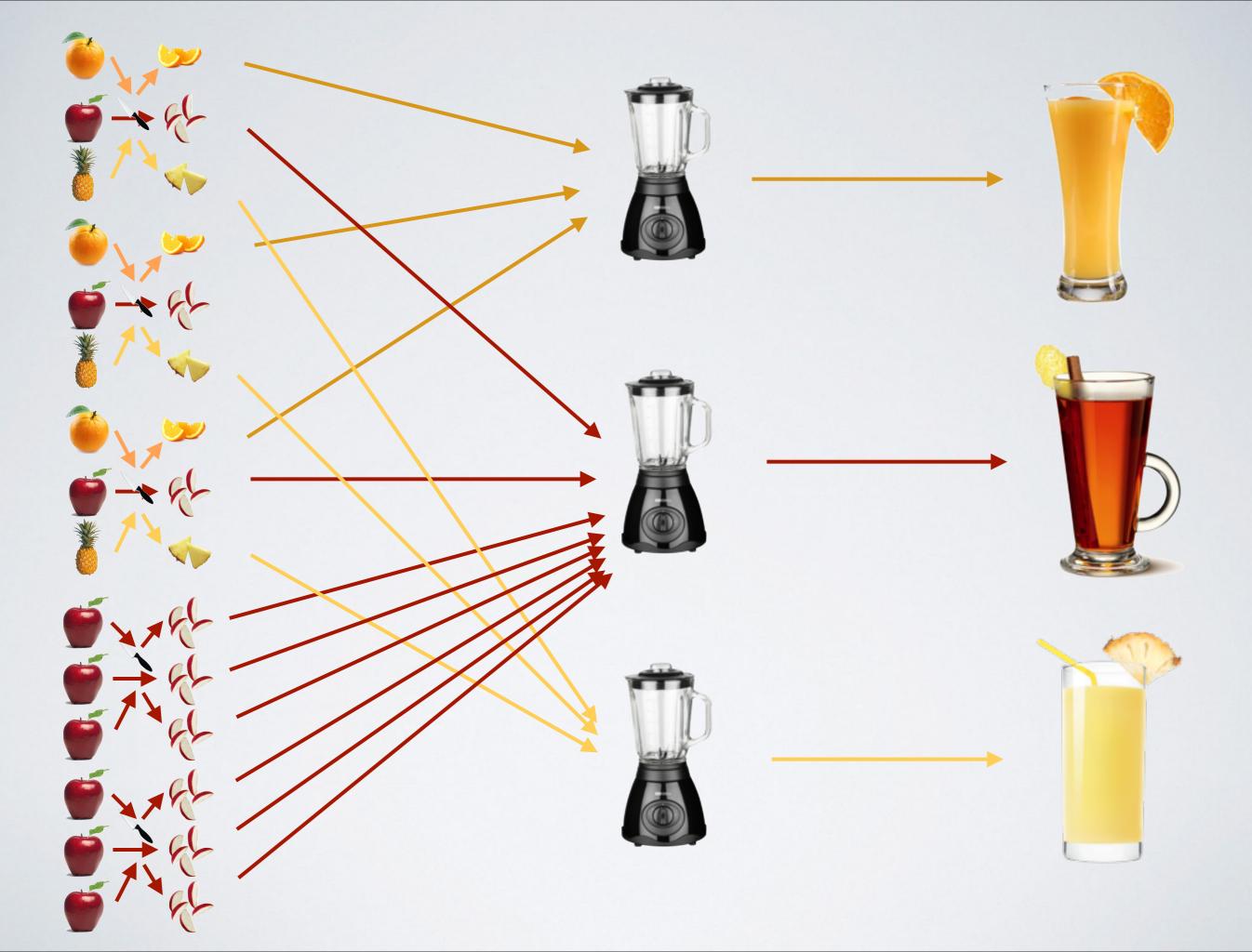


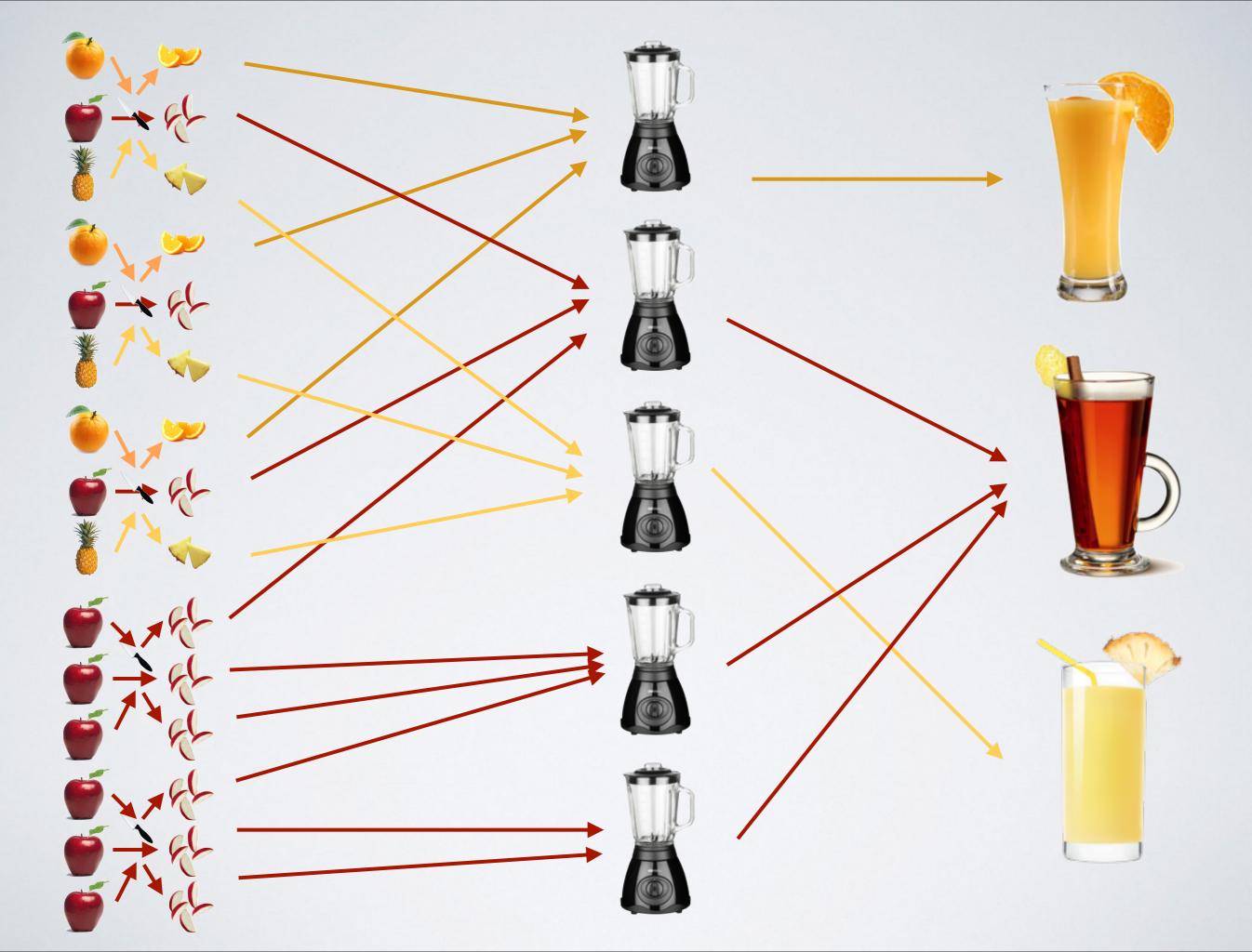


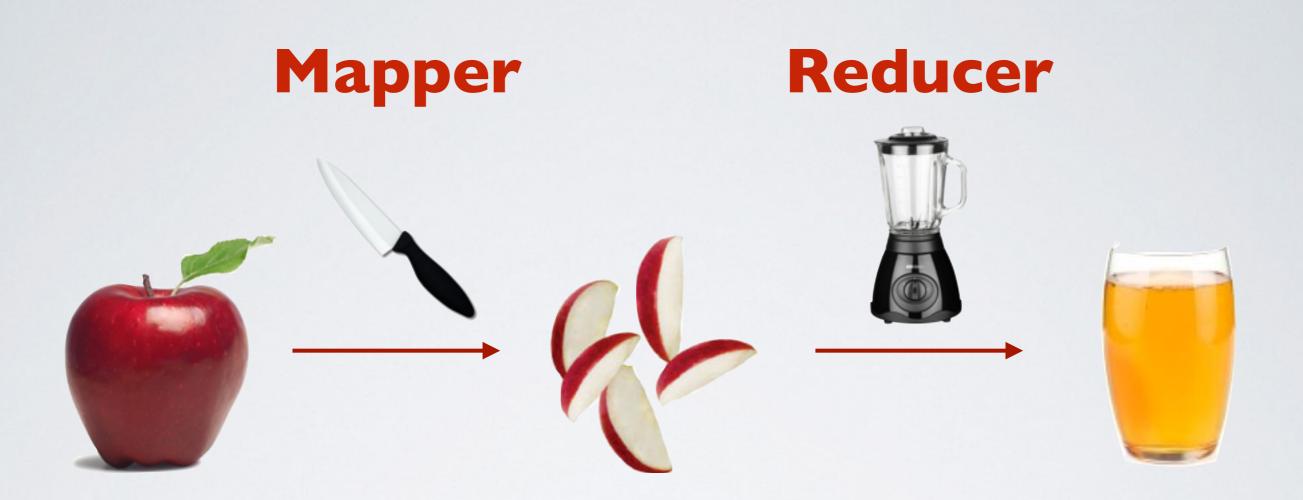












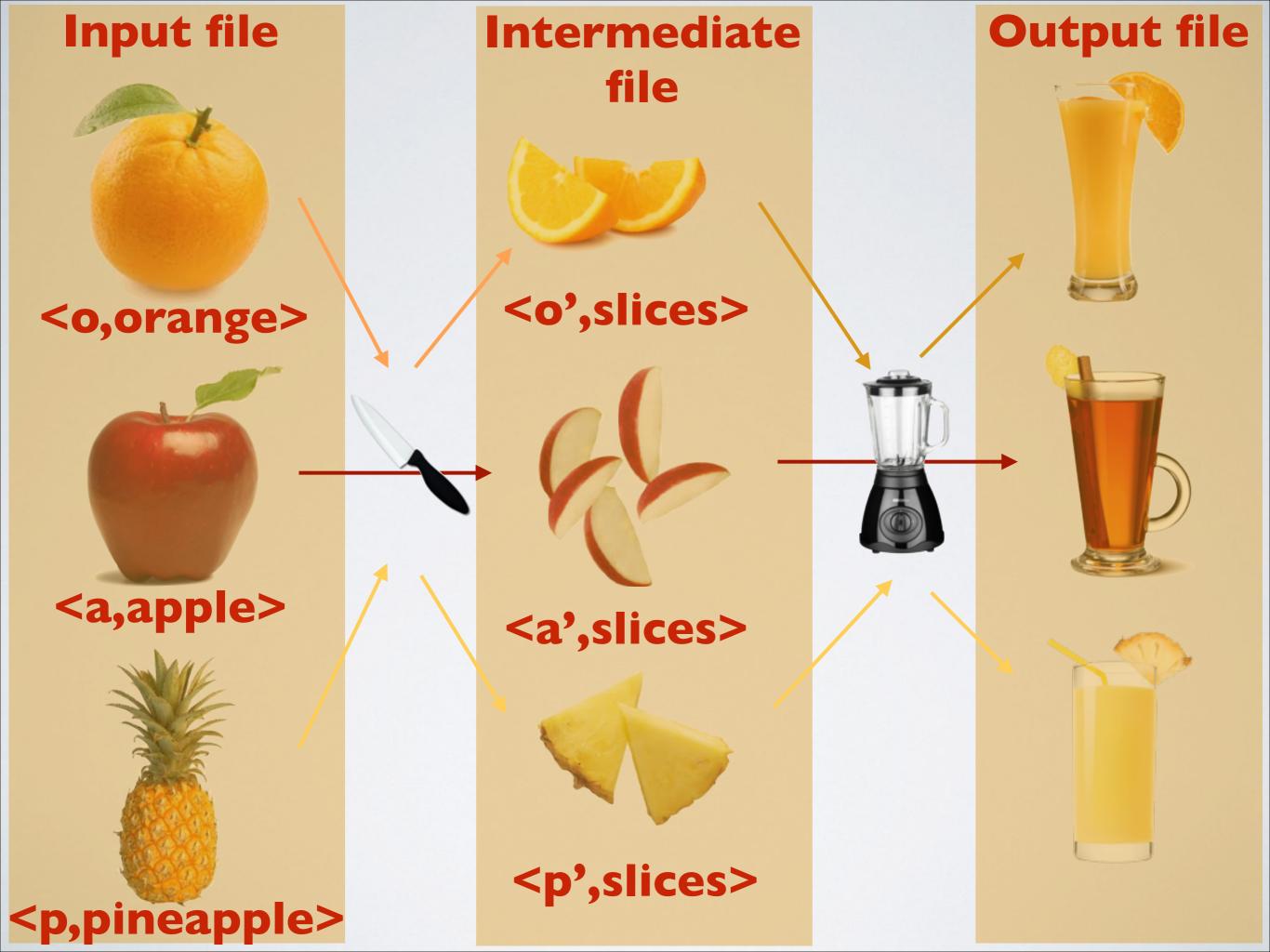
Input file

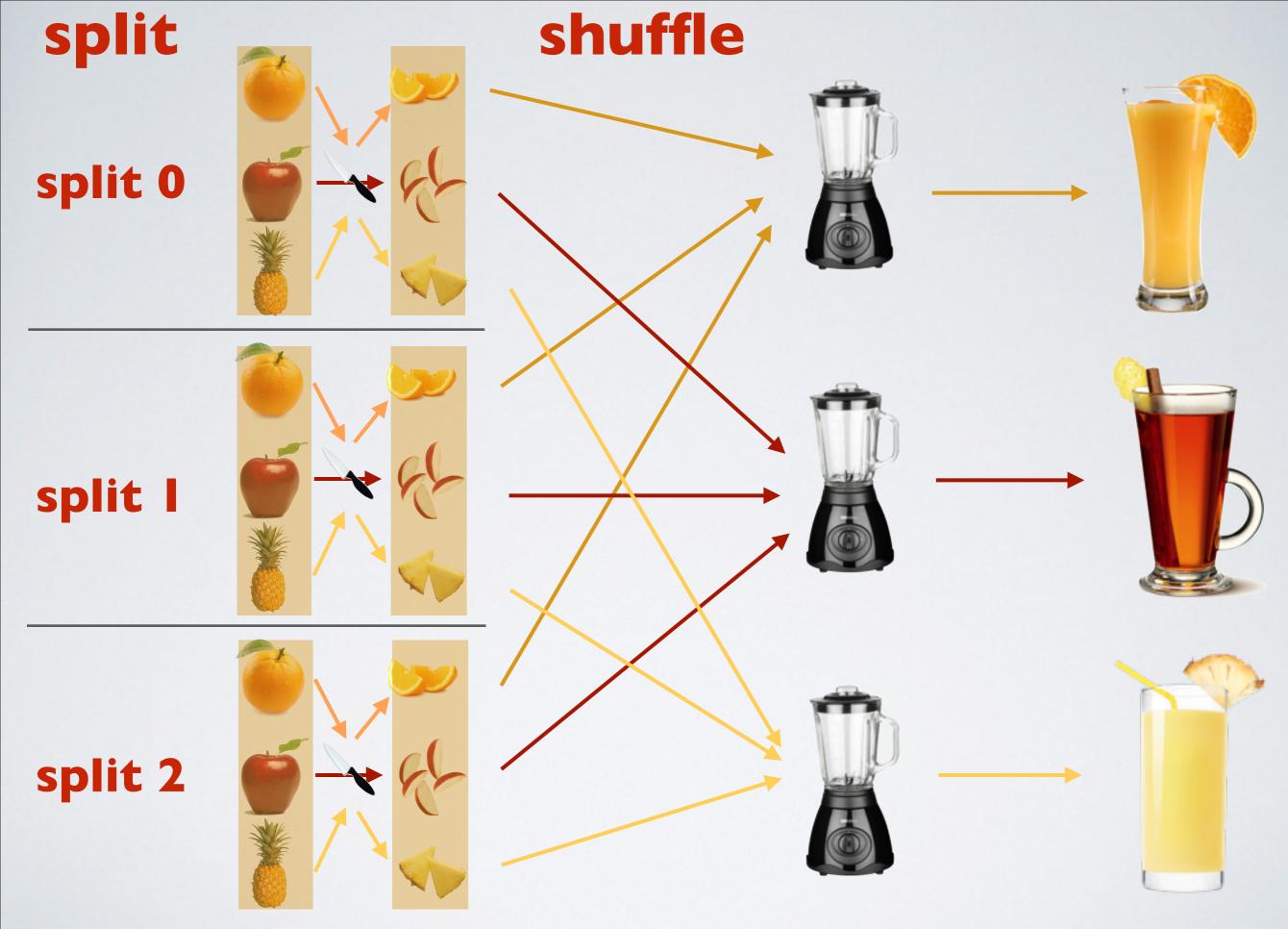
Intermediate file (local)

Output file

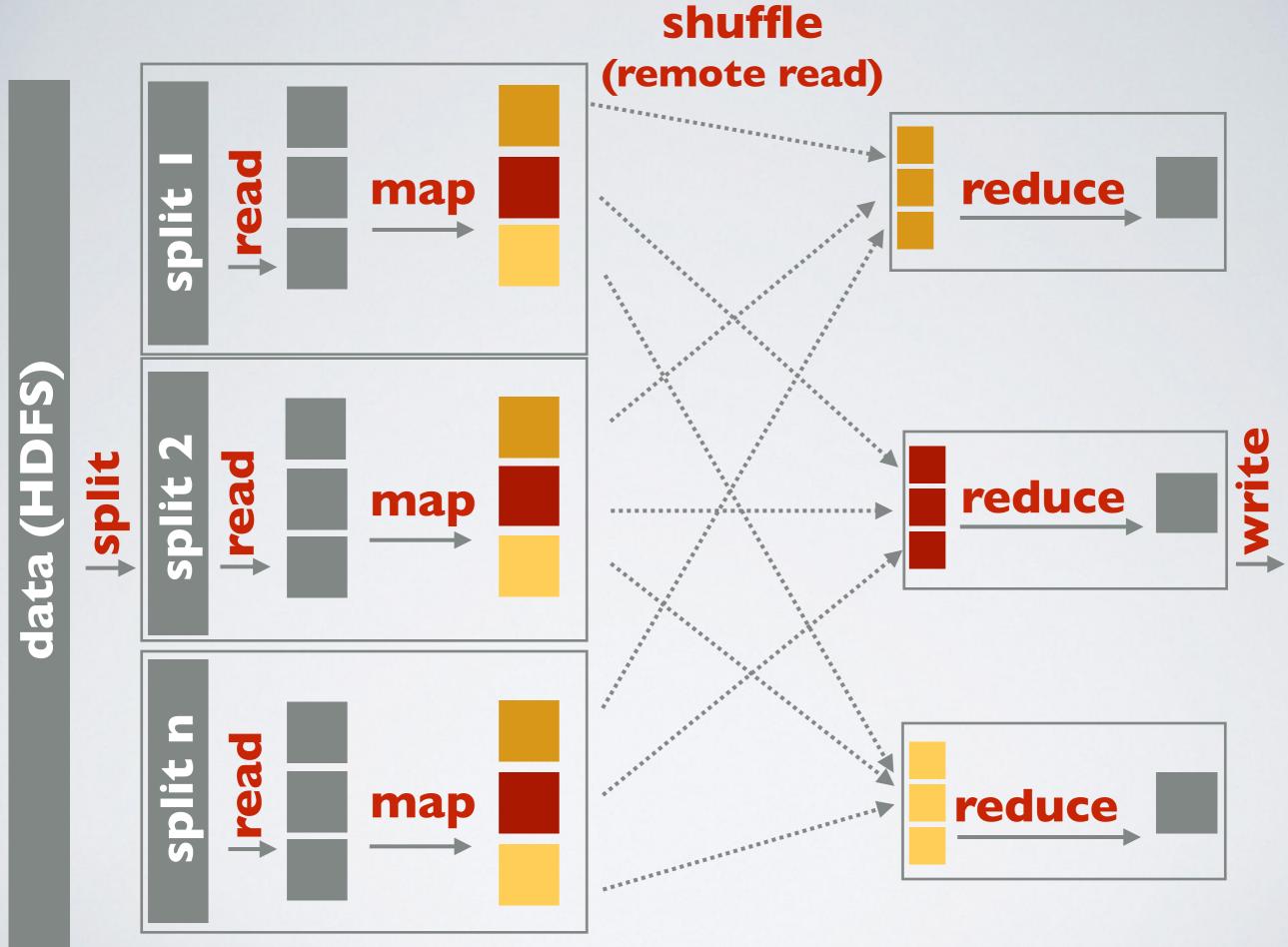
<a,apple>

<a',slices>





I mapper/split I reducer/key(set)

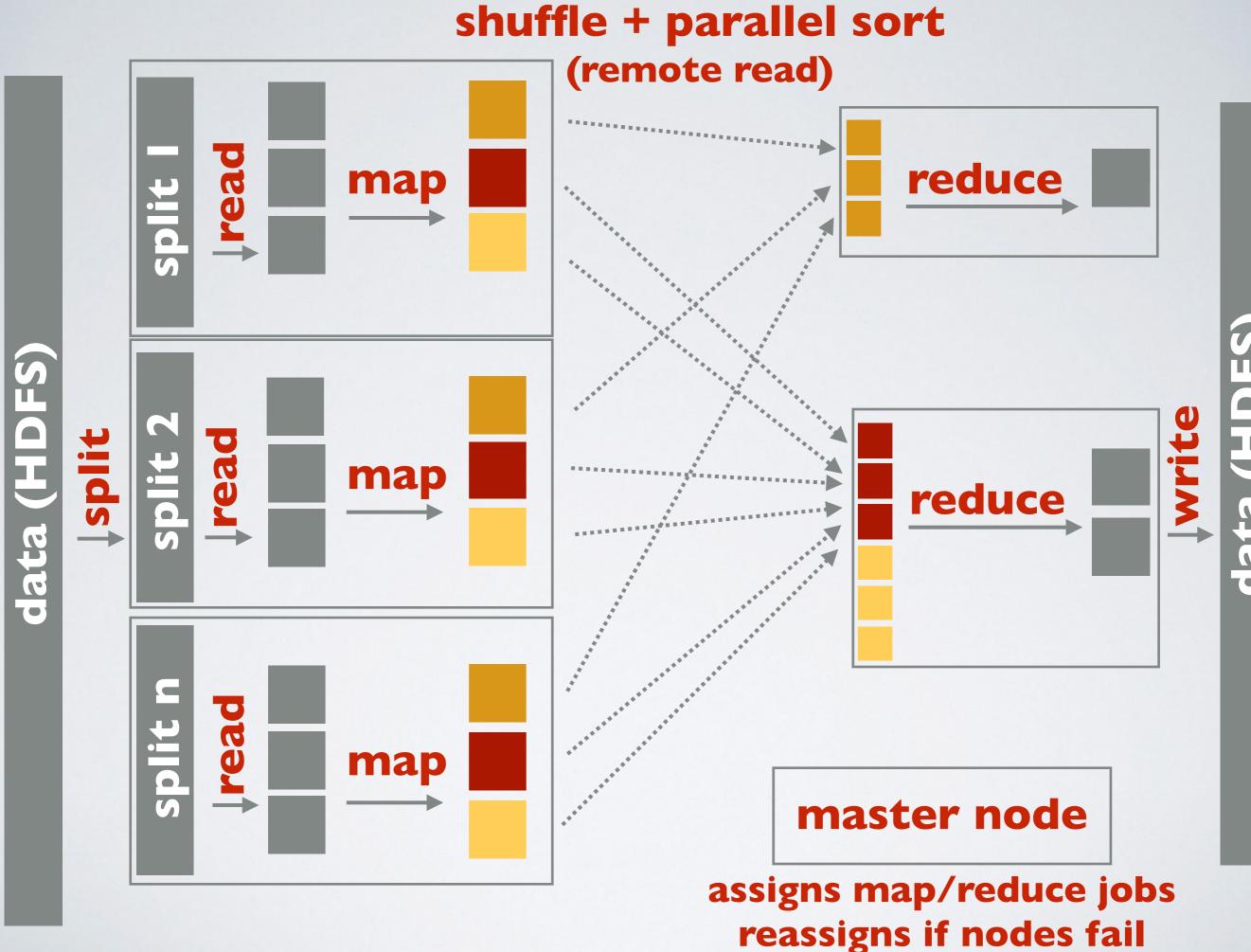


worker nodes (local)

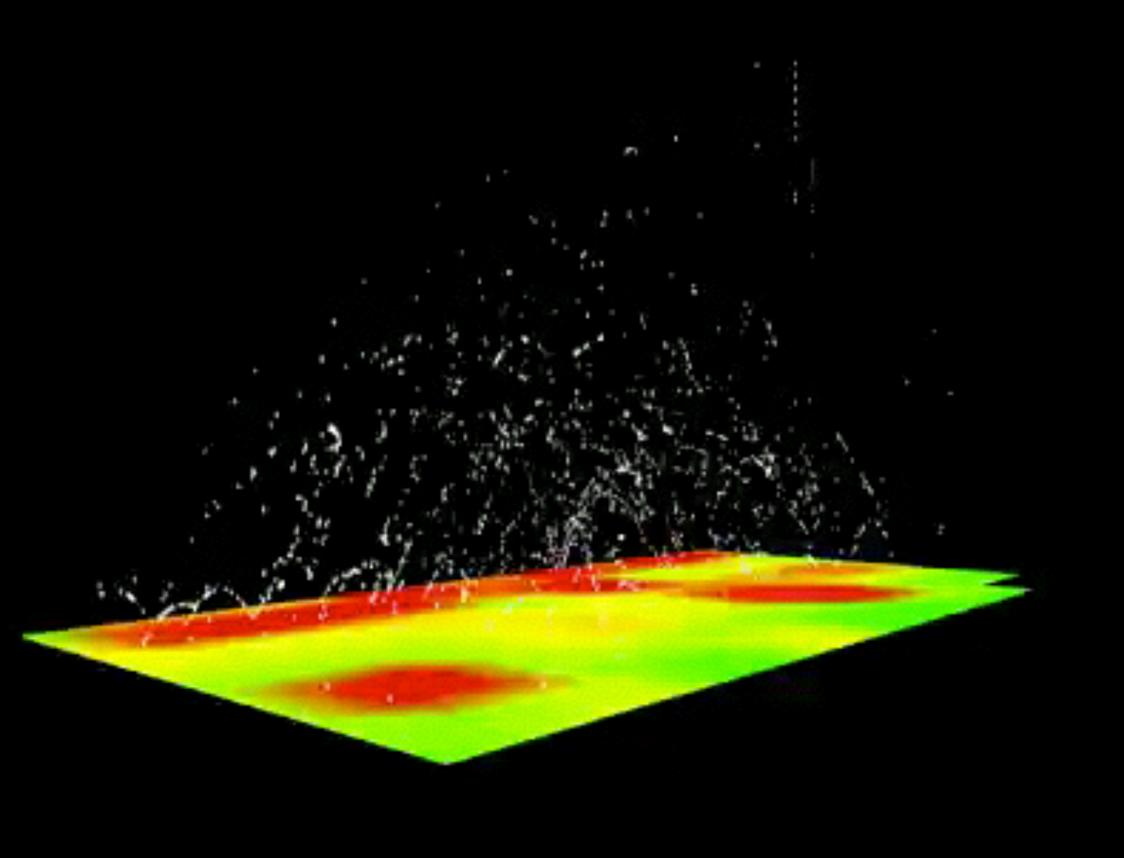
worker nodes (local)

(HDFS)

data



data



Google	chicken	Ļ	٩

chicken

Map phase (3 parallel tasks)

- $map_1 => ("why", (doc_1, 1)), ("did", (doc_1, 2)), ("the", (doc_1, 3)),$ ("chicken",(doc1,4)), ("cross",(doc1,5)), ("the",(doc1,6)), ("road",(doc1,,7))
- map₂ => ("the", (doc₂, 1)), ("chicken", (doc₂, 2)), ("and", (doc₂, 3)), ("egg",(doc₂,4)), ("problem", (doc₂,5))
- $map_3 => ("kentucky", (doc_3, 1)), ("fried", (doc_3, 2)), ("chicken", (doc_3, 3))$

Intermediate shuffle & sort phase

- ("why", <(doc1,1)>),
- ("did", <(doc1,2)>),
- ("the", <(doc1,3), (doc1,6), (doc2,1)>)
- ("chicken", <(doc1,4), (doc2,2), (doc2,3)>)
- ("cross", <(doc1,5)>)
- ("road", <(doc₁,7)>)
- ("and", <(doc₂,3)>)
- ("egg", <(doc₂,4)>)
- ("problem", <(doc₂,5)>)
- ("kentucky", <(doc₃,1)>)
- ("fried", <(doc₂,2)>)

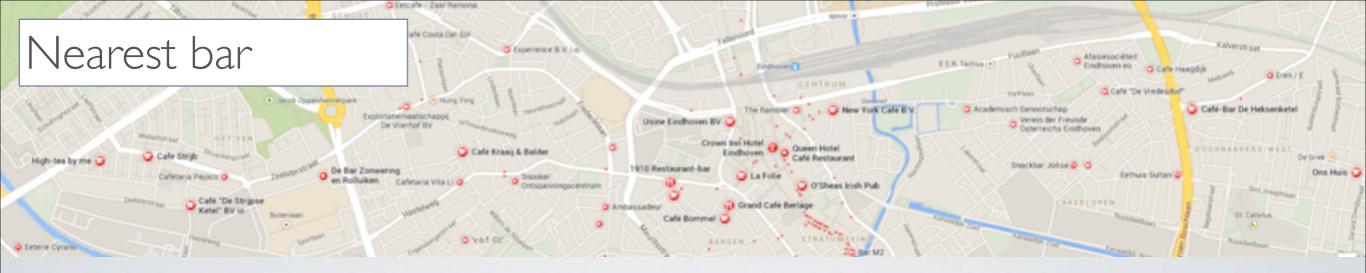
Google chicken

Intermediate shuffle & sort phase

- ("why", <(doc₁,1)>),
- ("did", <(doc₁,2)>),
- ("the", <(doc1,3), (doc1,6), (doc2,1)>)
- ("chicken", <(doc₁,4), (doc₂,2), (doc₃,3)>)
- ("cross", <(doc₁,5)>)
- ("road", <(doc₁,7)>)
- ("and", <(doc₂,3)>)
- ("egg", <(doc₂,4)>)
- ("problem", <(doc₂,5)>)
- ("kentucky", <(doc₃,1)>)
- ("fried", <(doc₃,2)>)

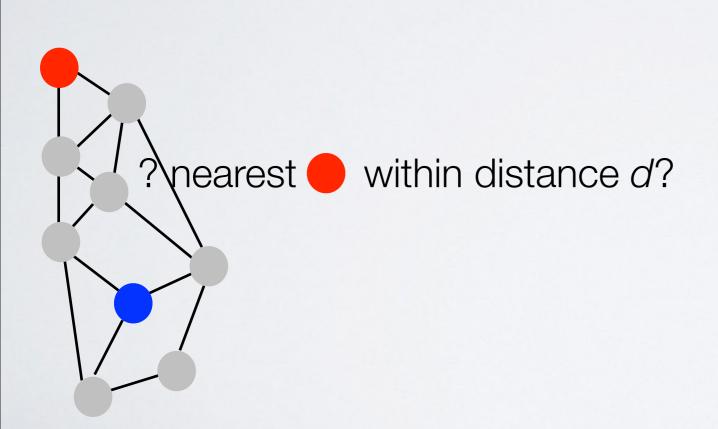
Reduce phase (11 parallel tasks)

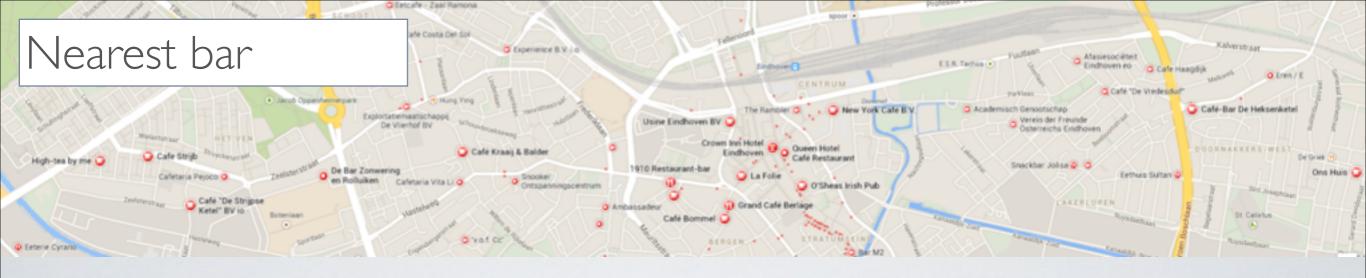
- ("why", <(doc₁,<1>)>),
- ("did", <(doc₁,<2>)>),
- ("the", <(doc₁, <3,6>), (doc₂, <1>)>)
- ("chicken", <(doc₁,<4>), (doc₂,<2>), (doc₃,<3>)>)
- ("cross", <(doc₁,<5>)>)
- ("road", <(doc₁,<7>)>)
- ("and", <(doc₂,<3>)>)
- ("egg", <(doc₂,<4>)>)
- ("problem", <(doc₂,<5>)>)
- ("kentucky", <(doc₃,<1>)>)
- ("fried", <(doc₃,<2>)>)



Input

graph (node,label)



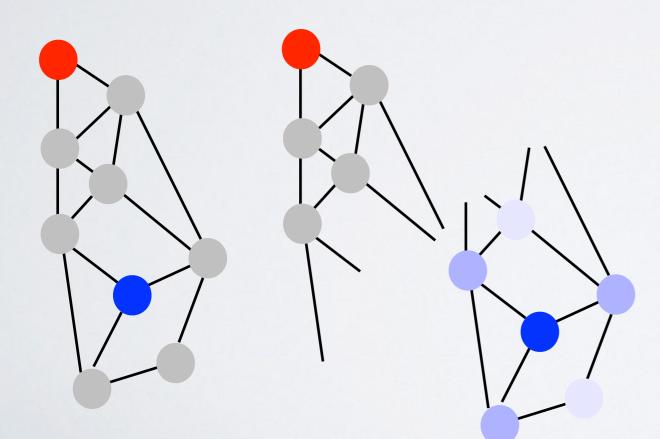


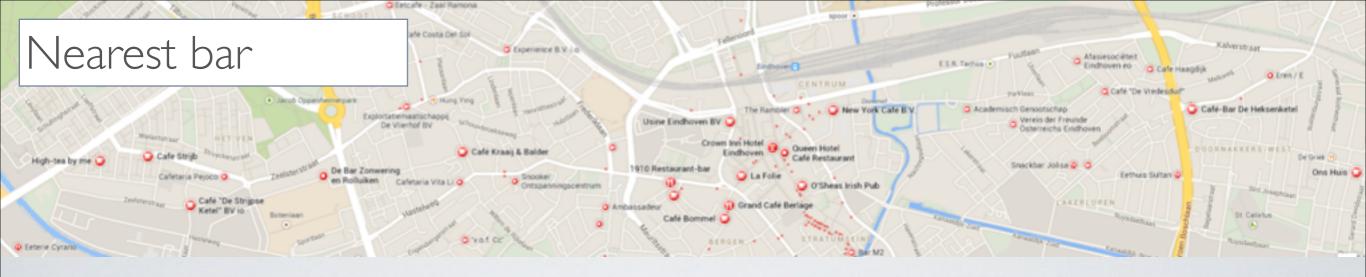
Input graph (node,label)

Мар

 $\forall \bullet$, search graph with radius d

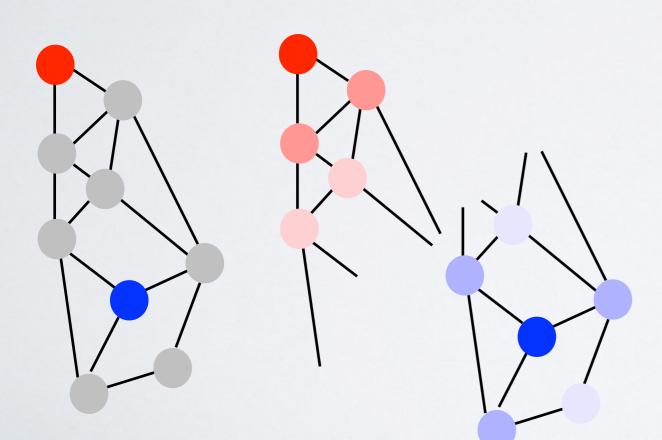
< _ ,{• ,distance} >

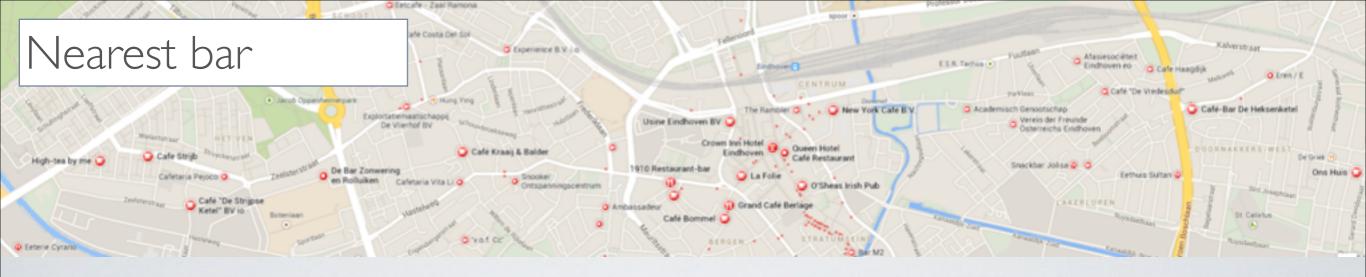




Input graph (node,label) Map
✓●, search graph
< _, {●, distance} >

Shuffle/ Sort by ●id





Input graph (node,label)

Map ∀●, search graph

by id

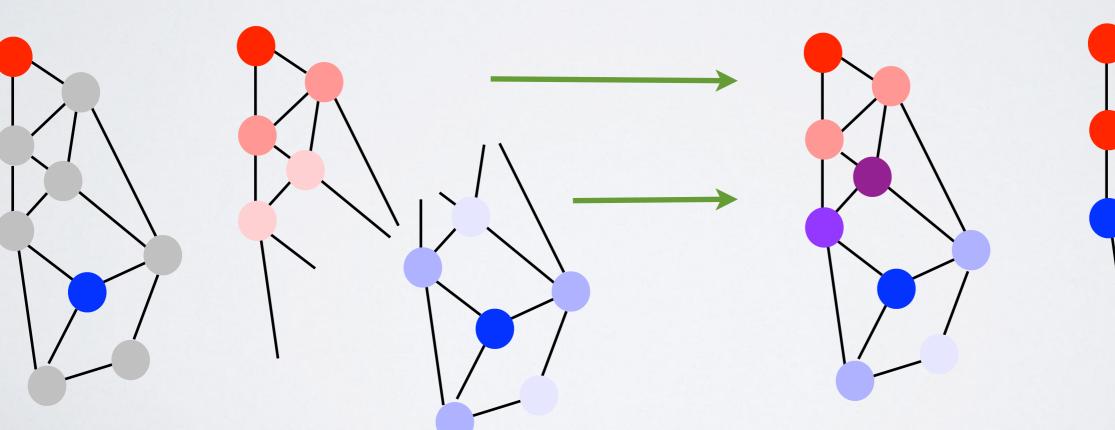
Shuffle/ Sort

< ,[{ , distance}, $\{ \circ, distance \} \} >$ -> min()

Reduce

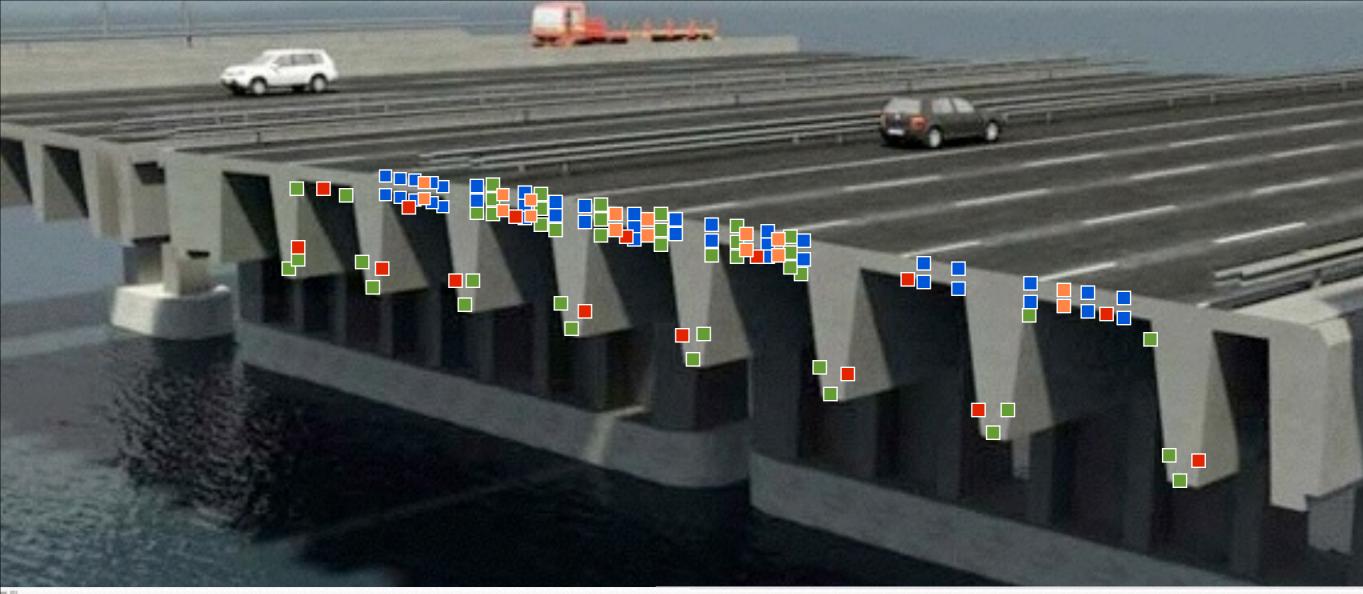
Output

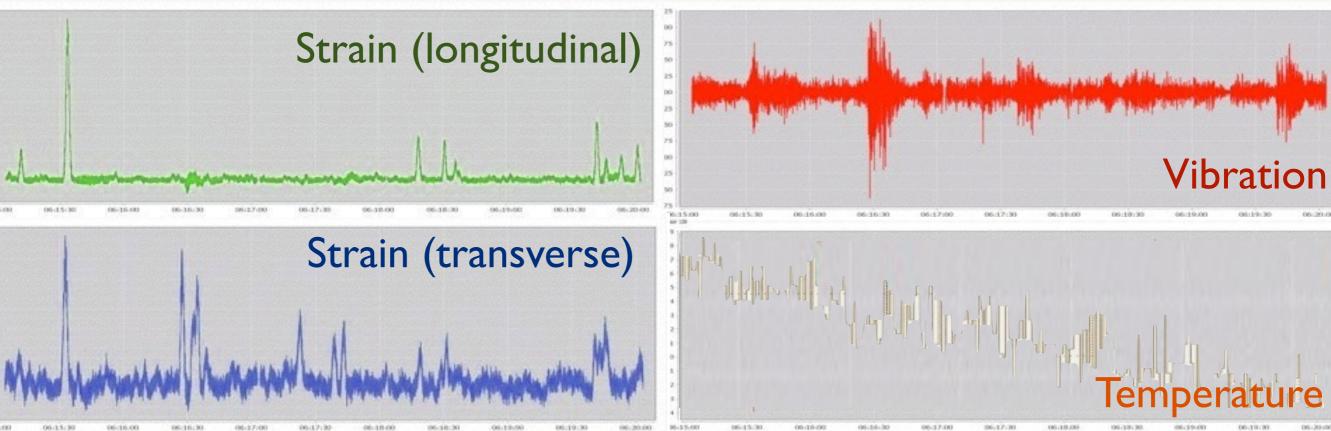
< , > < , > marked graph

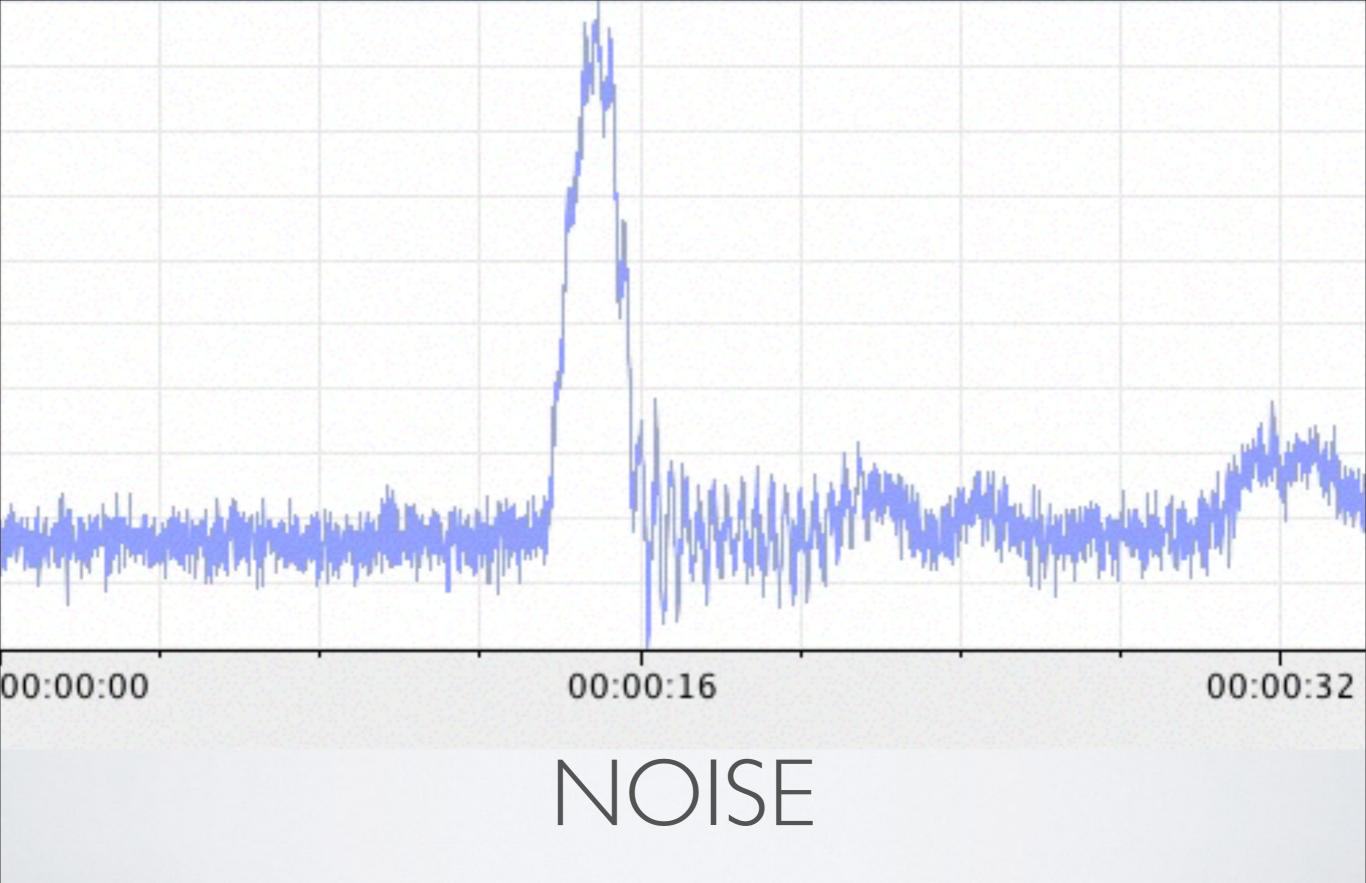


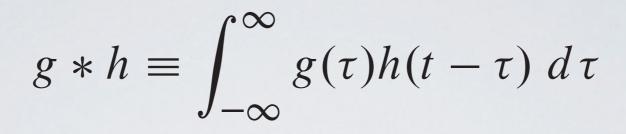
EXAMPLES

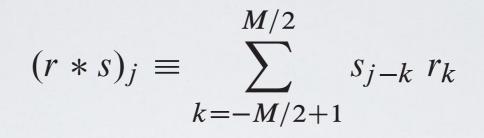
Sensor data

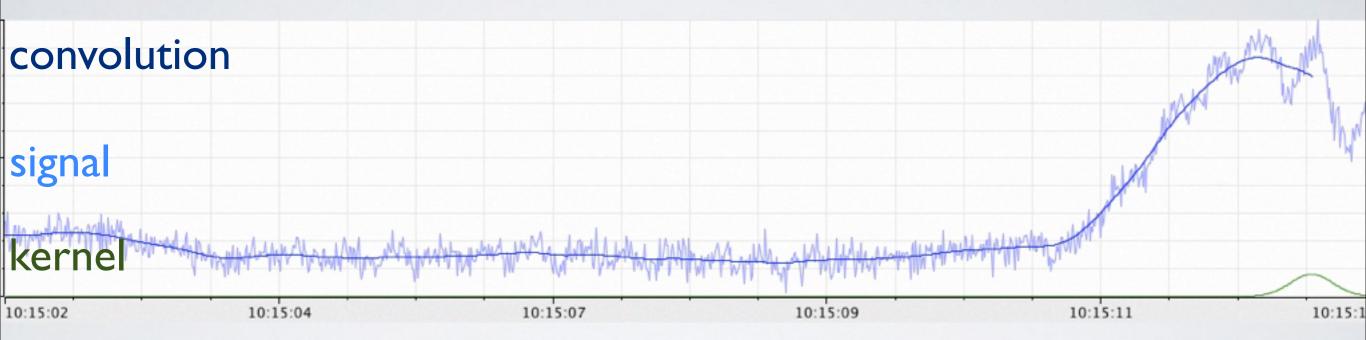












MATHS Convolution

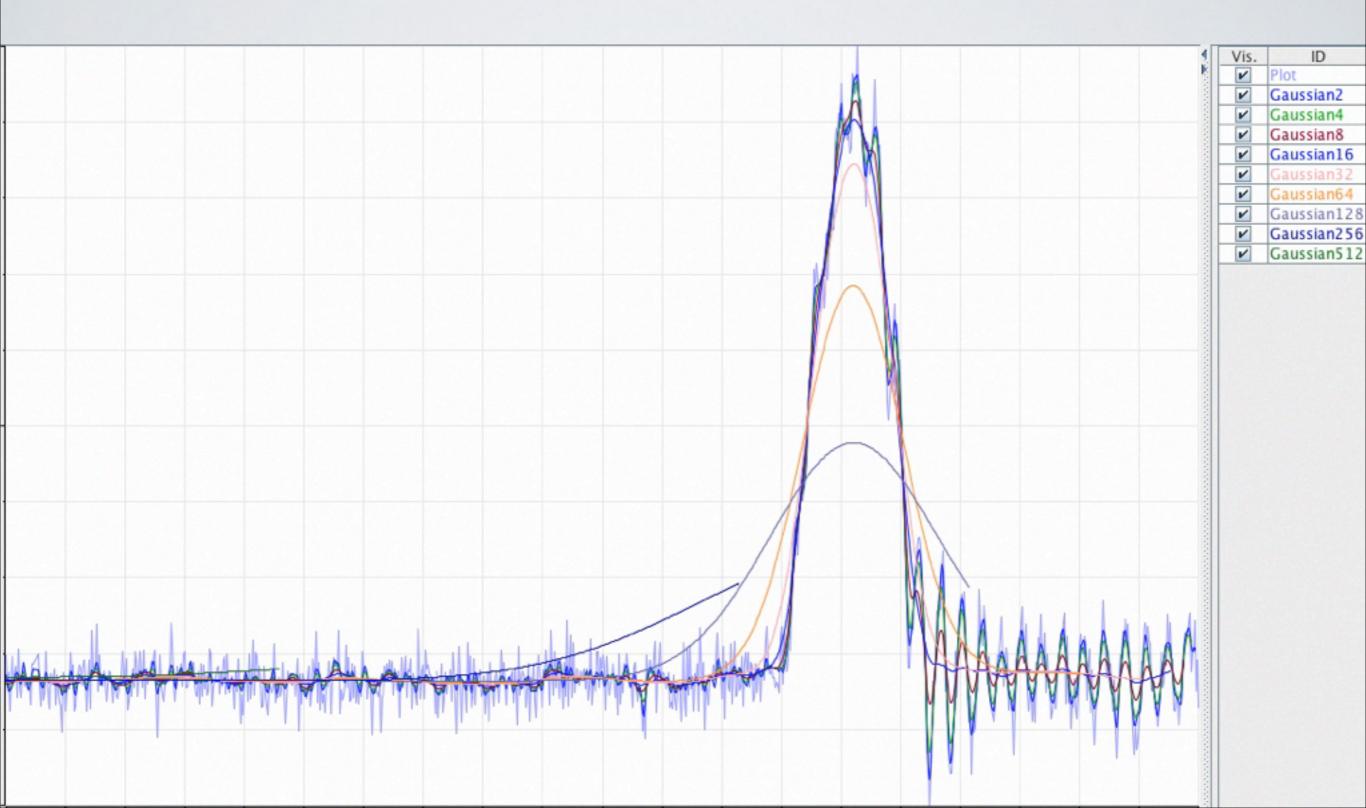
COMPLEXITY



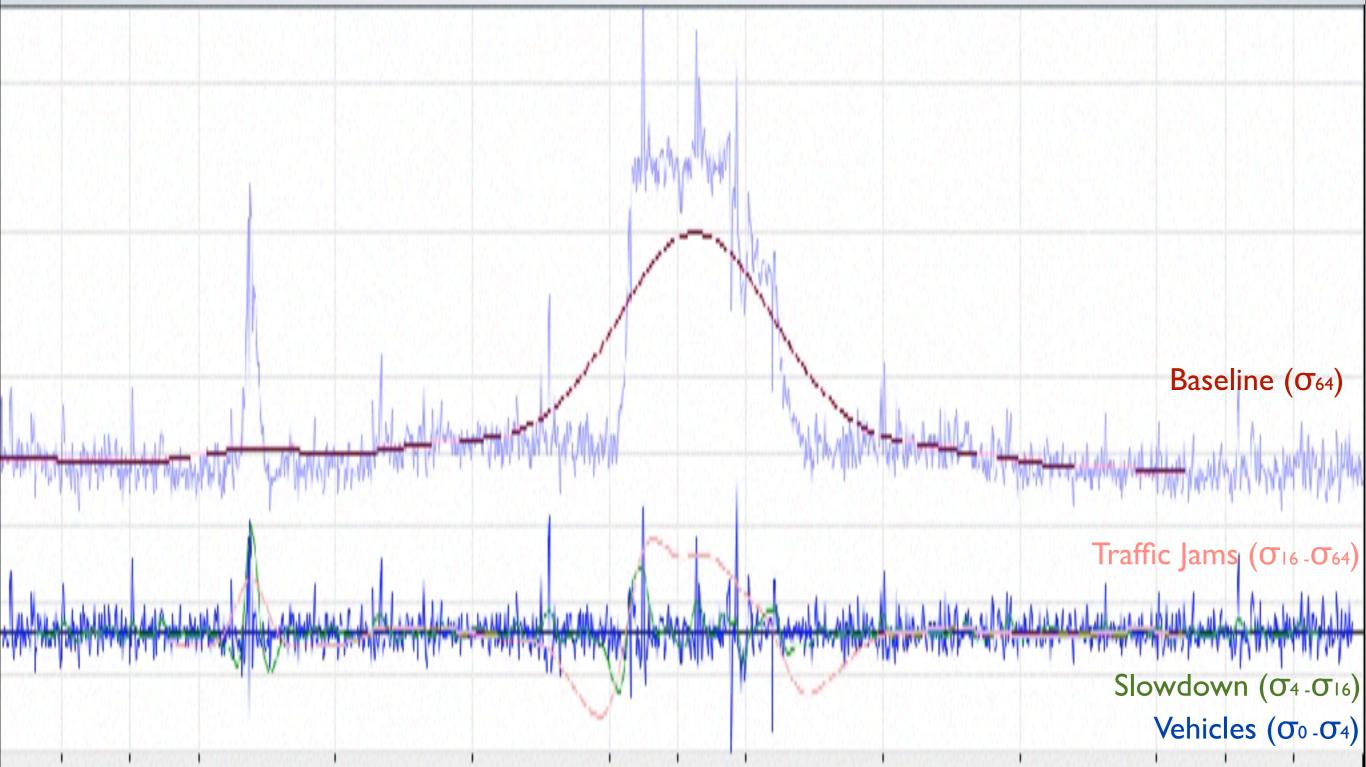
MATHS, AGAIN

scale space decomposition

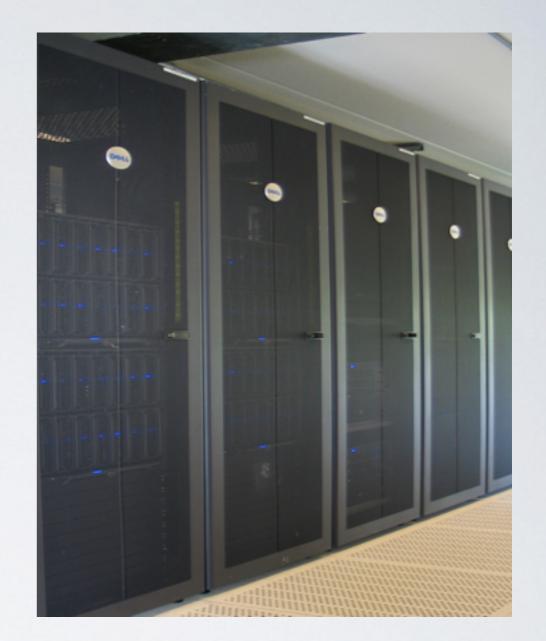
SCALE-SPACE



SCALE-SPACE DECOMPOSITION

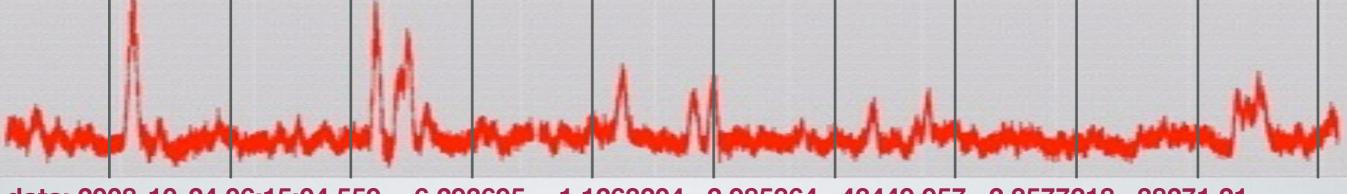


145 sensors 100Hz5GB/day 2TB/year 50MB/s disk I/O



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("\t");
    Text time = new Text(values[0]);
    for(int i = 1; i <= nrStressSensors; i++)
        context.write(time, new Text(values[i]));

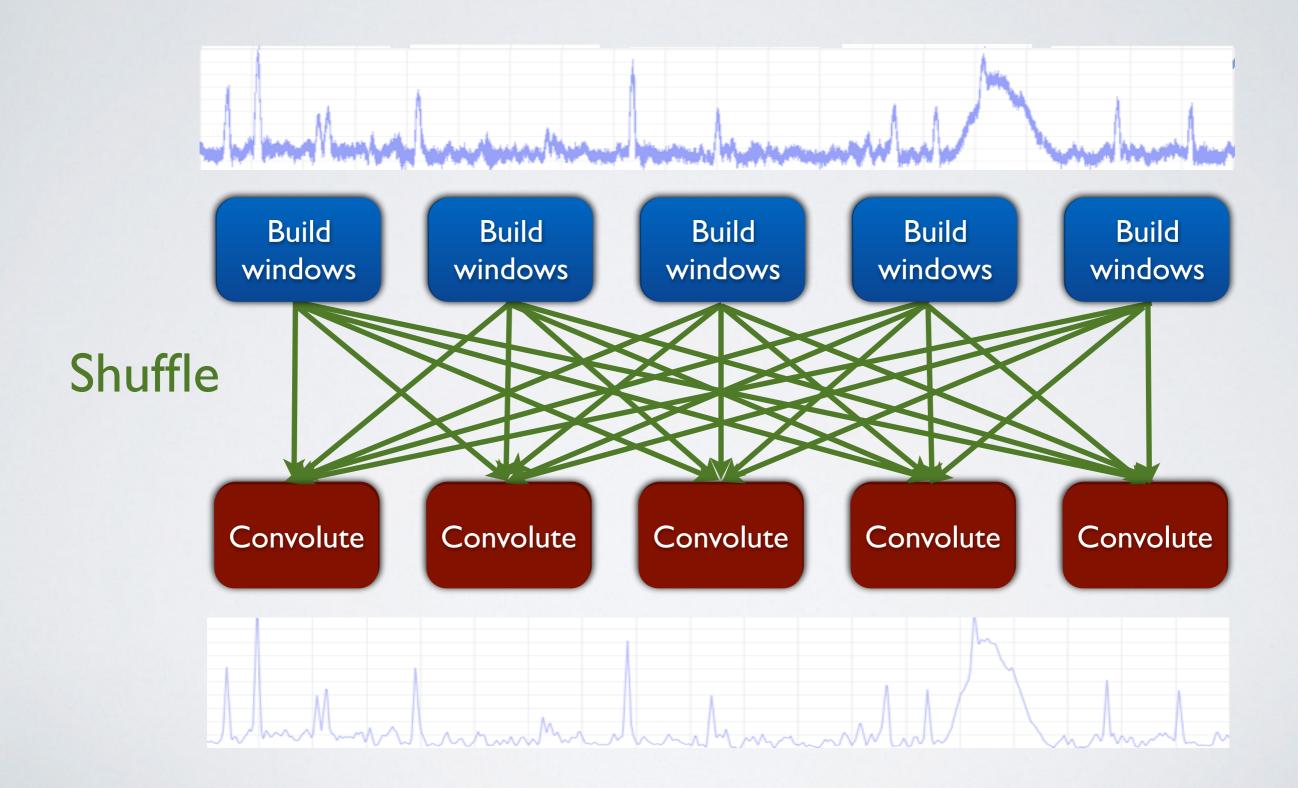
public void reduce(Text key, Iterable<Text> values, Context context) {
        //init; sum, min, max, count = 0
        Double d;
        for (Text v : values) {
            d = Double.valueOf(v.toString());
            sum += d;
            rein = Math min(min_d);
        }
    }
}
```

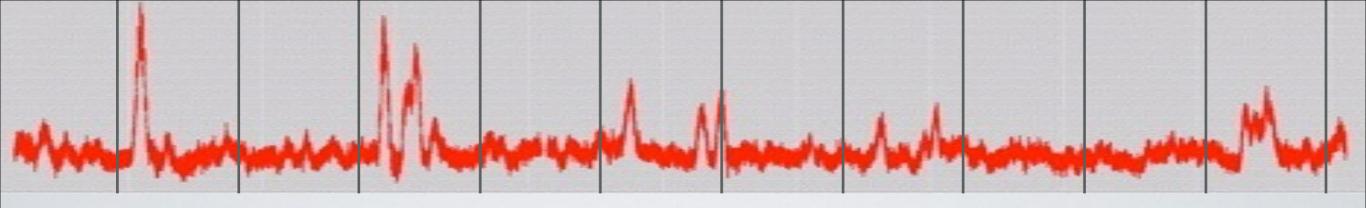
min = Math.min(min, d); max = Math.max(max, d);

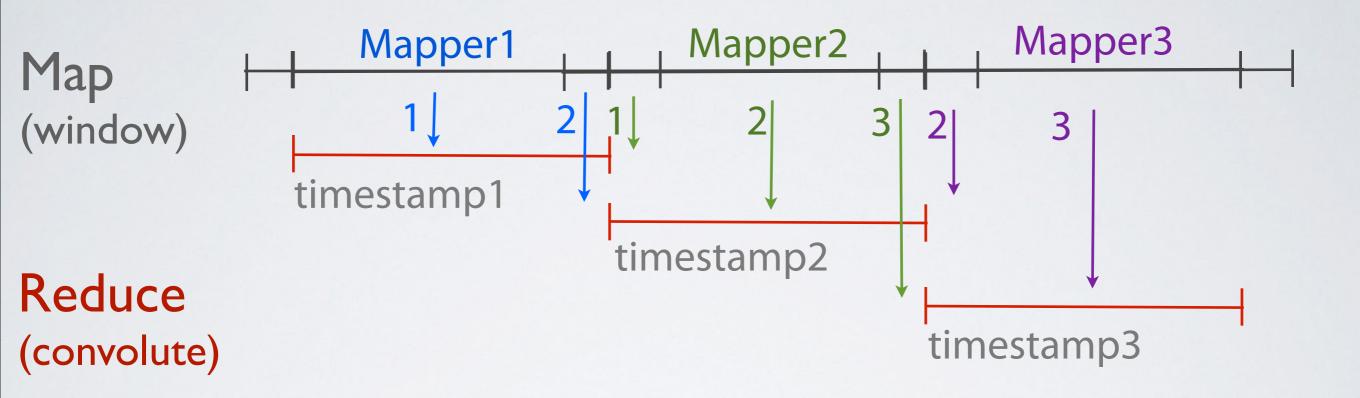
count++;

```
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

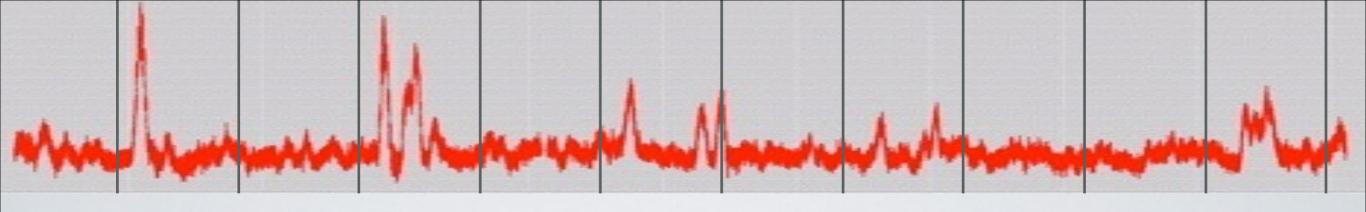


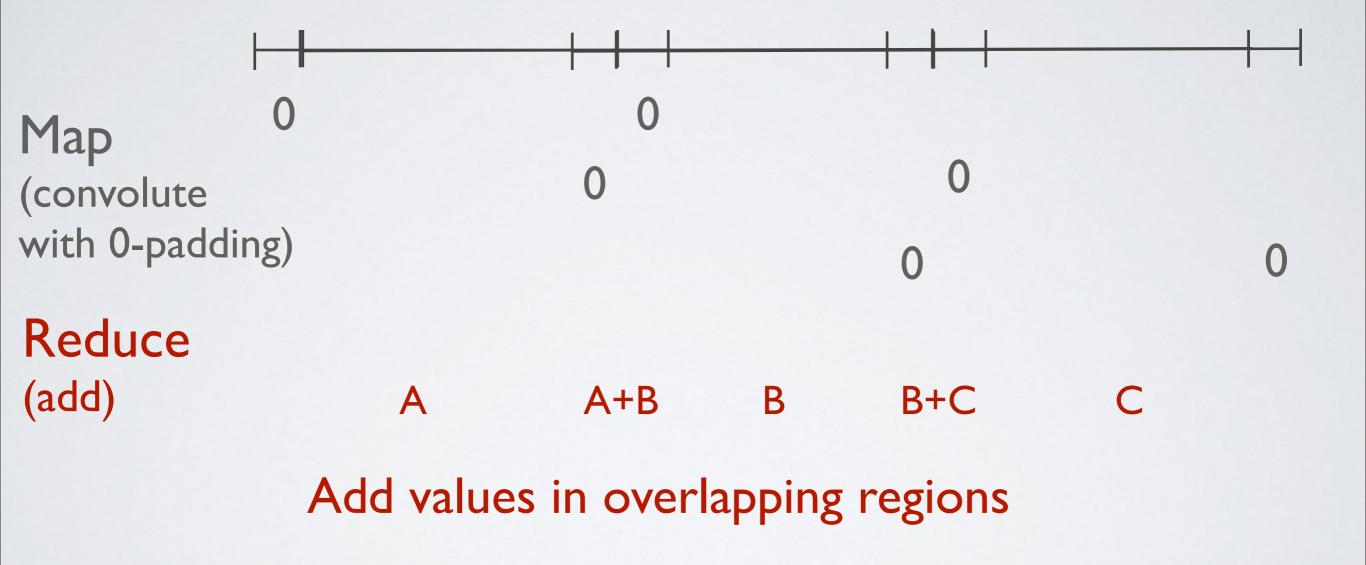




Emit only unpolluted data

OVERLAP-CONVOLUTE

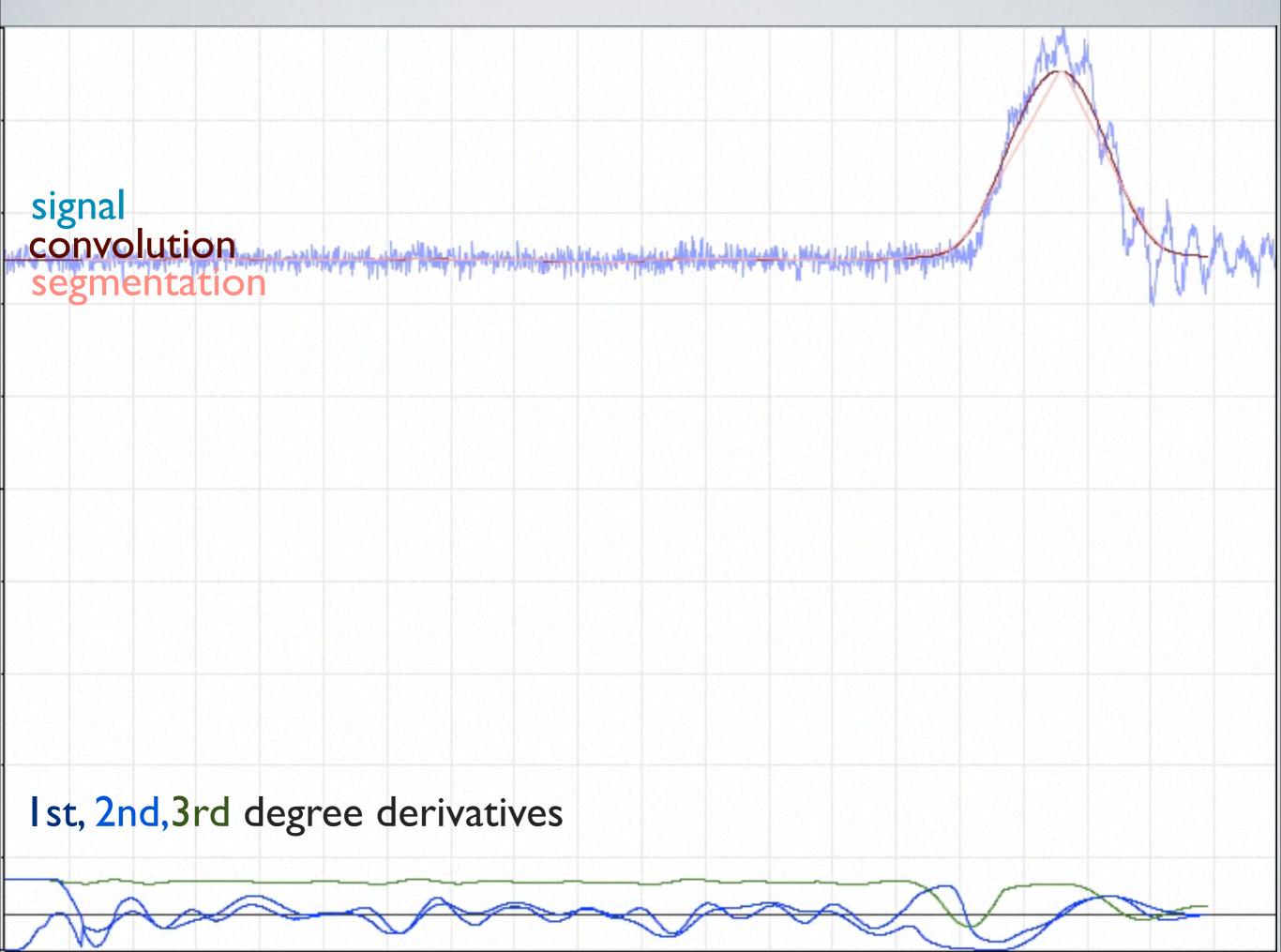




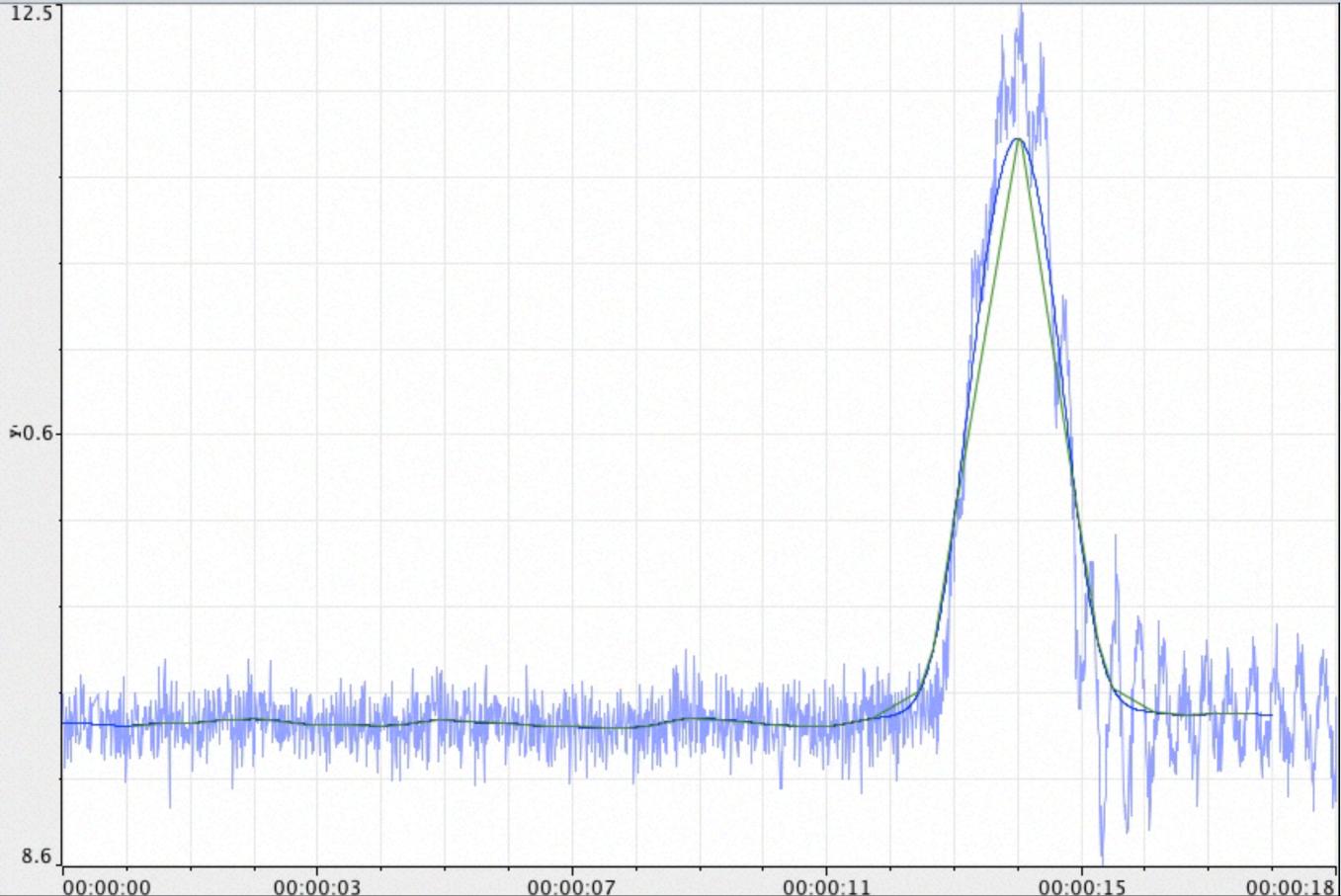
CONVOLUTE-ADD

SEGMENTATION

- You don't need 100Hz data for everything
- Approximate signal with linear segments
- Key points: 0-crossings of 1st, 2nd, 3rd derivative
- Maths: derivative of smoothed signal = convolution with derivative of kernel







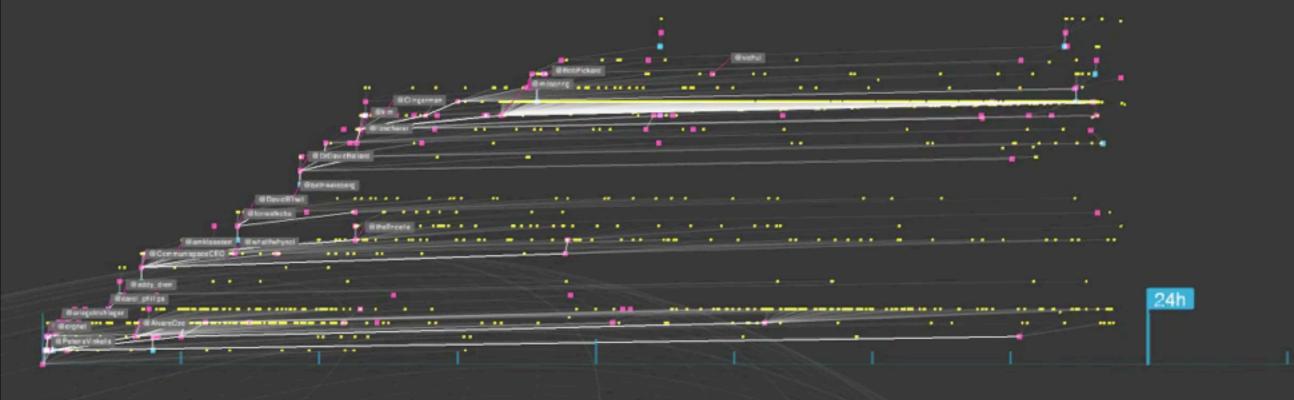


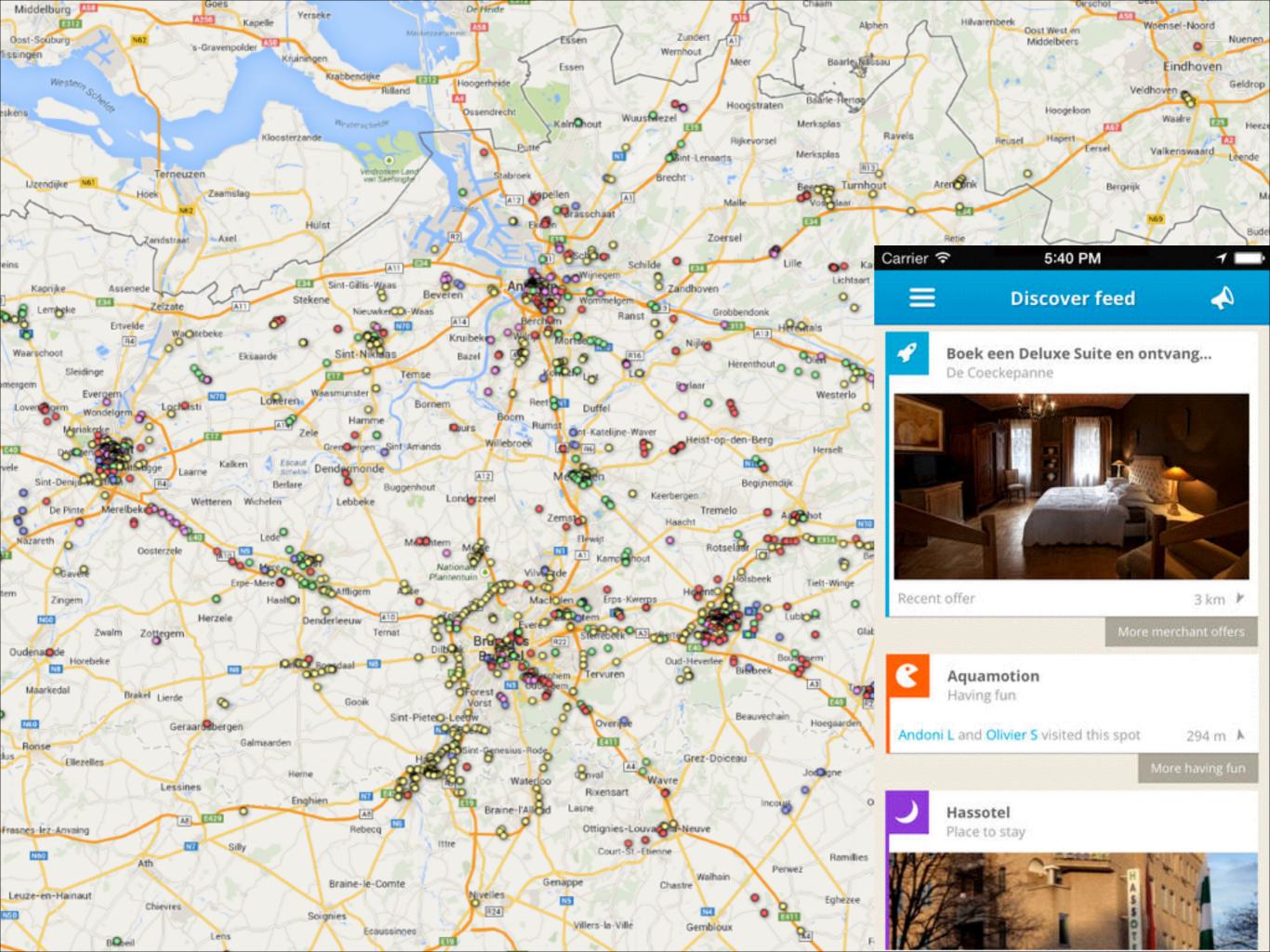
TRACKING NEWS STORIES



But Will It Make You Happy? By STEPHANIE ROSENBLOOM Mon Aug 09 10:46:09 EDT 2010







6AM New York City

Residence

Food

Arts & Entertainment

College & University

Nightlife Spot

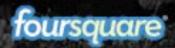
Great Outdoors

Shop & Service

Professional & Other Places

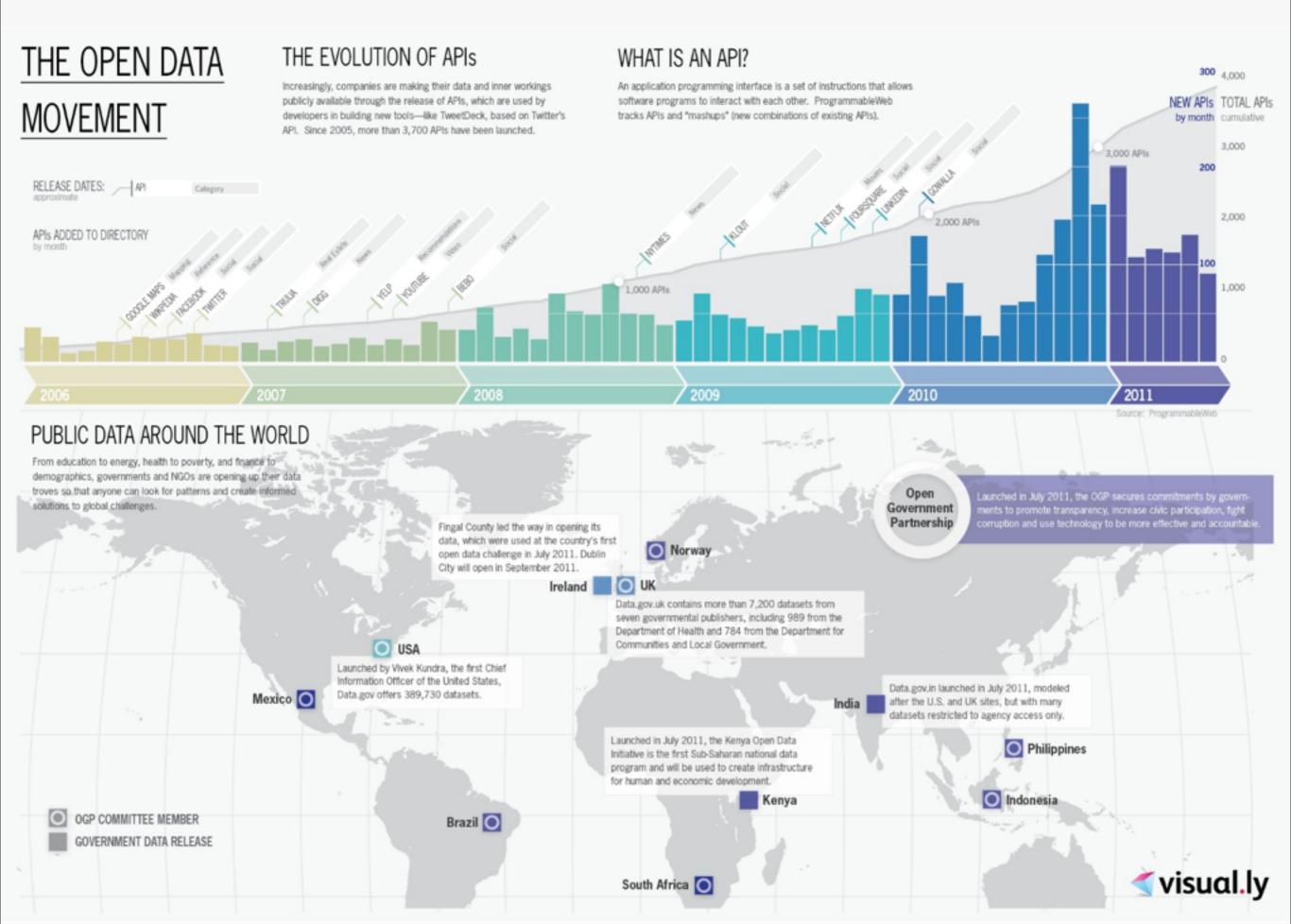
Travel & Transport

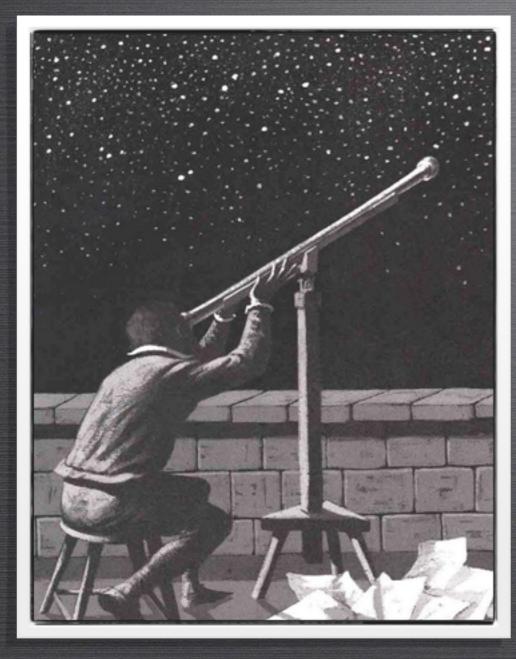
Geospacial data





OPEN DATA OPEN SCIENCE

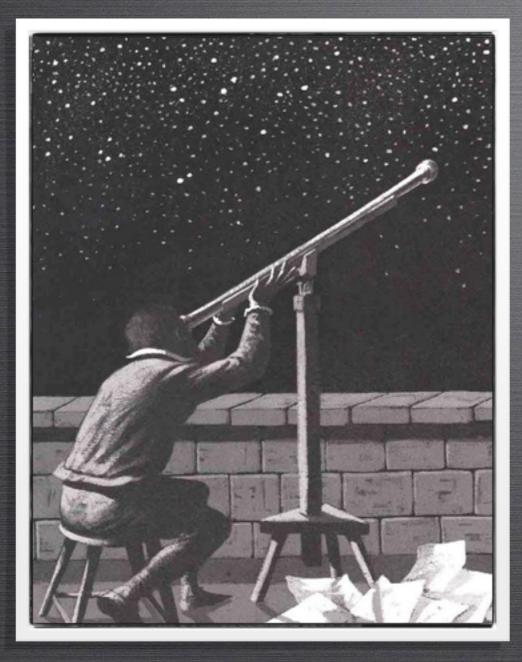




1609

GALILEO GALILEI DISCOVERS SATURN'S RINGS

WHAT DID HE DO?



1450

PRINTING PRESS

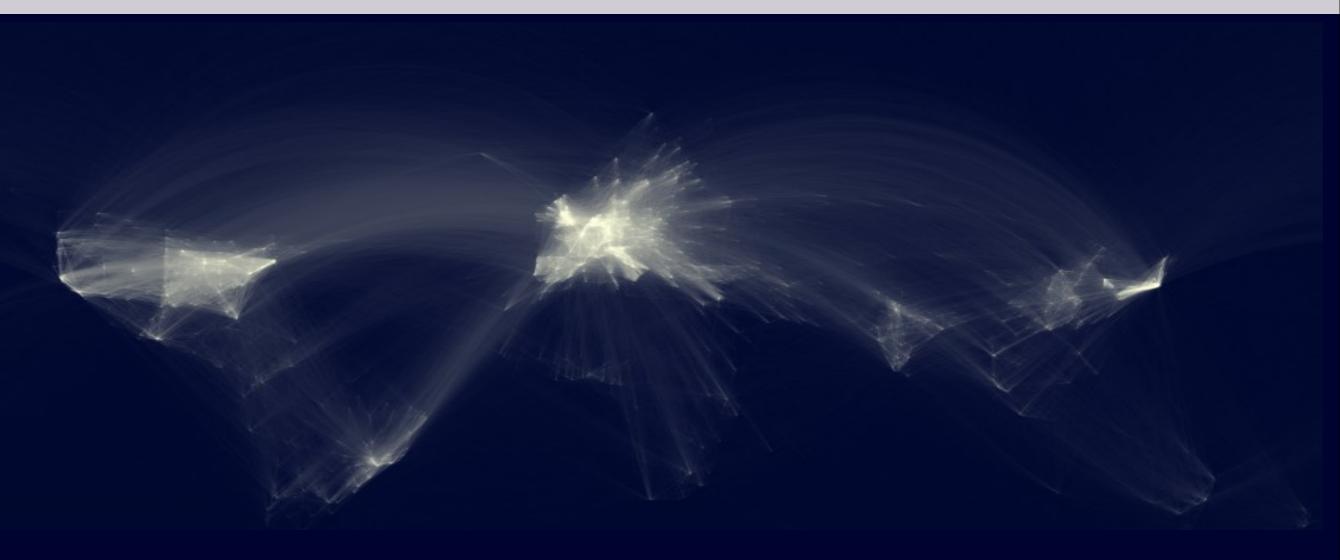
1609 Galileo Galilei ANAGRAMS

18TH CENTURY

SCIENTIFIC REVOLUTION

JOURNAL ACCEPTED AS BEST WAY TO ADVANCE SCIENCE

today



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

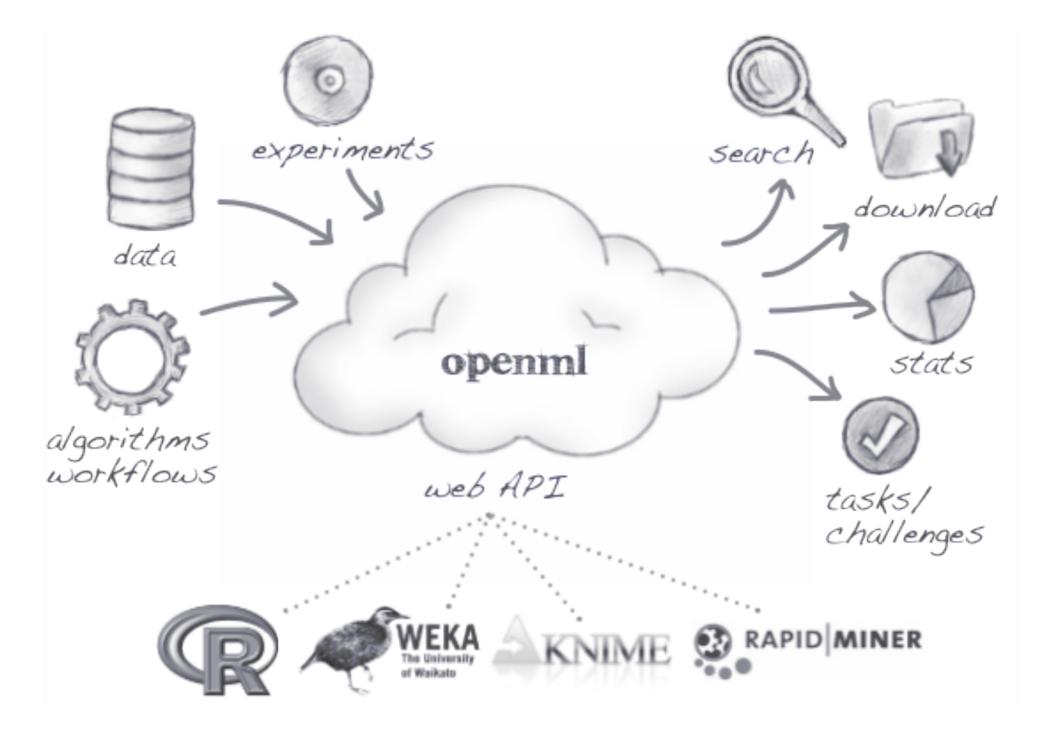


Search 575889 experiments on 130 datasets and 191 algorithm/workflow implementations

openml.org

Share results

Search results



Integrated in machine learning tools

Search: Free text

	OpenML	Search	Share	Plugins	Developers	s Comr	nunity 🖀 Sign	i in	y in	§ † f	
Q All	I Datasets	📽 Implement	ations	I Metrics	🗹 Tasks	7 Runs	Advanced	🖋 SQL	🖞 Graph	I Results	
Search tree	ı								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

🔲 tic-tac-toe

1. 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

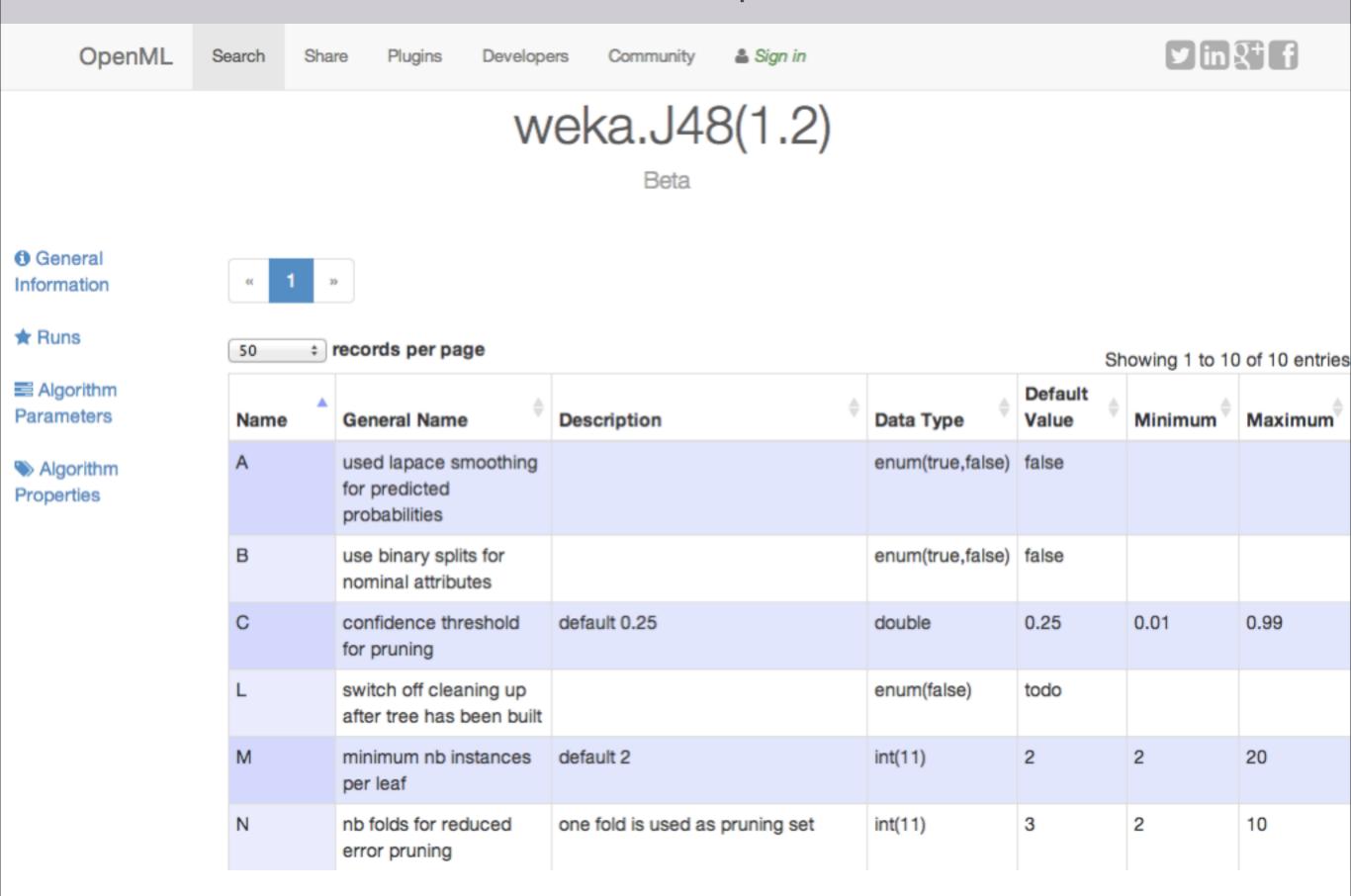
Search: Algorithm detail

OpenML	Search	Share Plugins	Developers	Community	🛔 Sign in			¥ in ₹†	0	
			wek	a.J48 Beta	3(1.2)					
 General Information 	Use	the dropdown be	low to select which	evluation me	asure should be used					
★ Runs Algorithm Parameters	predic Copy	tive accuracy Print CSV	¢ PDF					S	earch:	
		Name				\$	Evaluation		$\frac{1}{2}$	
Algorithm Properties	0	anneal					0.984409987	926483		
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	0	kr-vs-kp	kr-vs-kp				0.994368016719818			
	0	labor					0.736841976	642609		
	0	arrhythmia								
		arriyumia	1				0.6438050270	008057		
	0	letter	1				0.6438050270			
			1					648407		
	۲	letter					0.879800021	648407 243469		

Search: Run detail

OpenML	Search	Share	Plugins	Developers	Community	🛔 Sign in			Ƴ in § † f
				wel	ka.J48 Beta	3(1.2)			
 General Information 	Us	e the dro	opdown be	olow to select which	ch evluation me	asure should be	used.		
★ Runs Algorithm Parameters	Algorithm Copy Print CSV PDF								
T di di liotoro			Name				Å.	Evaluation	*
Algorithm Properties	•		anneal					0.984409987	926483
		Paramet C M R	er Name	Description confidence thresh minimum nb insta use reduced error	ances per leaf		Chosen value 0.25 2 false		
	0		anneal.Ol	RIG				0.909799993	038177
	0		kr-vs-kp					0.994368016	719818
	0		labor					0.736841976	642609
	0		arrhythmi	а				0.643805027	008057

Search: Algorithm parameters



Search: Algorithm properties

OpenML	Search Share Plugins Dev	velopers Community 🏝 Sign in	ש in פָּ+ָ f		
		weka.J48(1.2) Beta			
 General Information Runs 	 « 1 » 50 ÷ records per page 		Showing 1 to 12 of 12 entries		
Algorithm	Name	Description	Showing 1 to 13 of 13 entries		
 Parameters Algorithm Properties 	BiasVarianceProfile	The weight of the bias component in the learning algorithm's error. I.e., the percentage of errors that can be attributed to bias error (underfitting) as opposed to variance error (overfitting).	0.67804121865815		
	BiasWeightKohaviWolpert	empirically calculated average ratio of bias error in the total error, using Kohavi-Wolpert's definition of bias and variance	0.67804121865815		
	BiasWeightWebb	empirically determined average ratio of bias error in the total error, using Webb's definition of bias and variance	0.772941309061007		
	HandlesMissingValues		true		
	HandlesNominalFeatures		true		
	HandlesNominalTarget		true		
	HandlesNonBinaryClasses		true		
	HandlesNumericFeatures		true		

Search: Dataset detail

OpenML	Search	Share	Plugins	Developers	Community	🛎 Sign in	y in ₹† f
					iris Beta		
General Information	-	-		-	-	re shown. Press the "Show all/best resul ure should be used.	ts" button to include all results.
★ Runs	predictive	20011201		\$			
Data Features			CSV PDF		t results		Search:
Solution Data Properties		Impler	mentation		\$	Algorithm $ eqtilde{} eqti$	Evaluation
	0	weka.	MultilayerPe	erceptron(1.2)		MultilayerPerceptron	0.980000019073486
	٢	weka./	AdaBoostM	1(1.24.2.3)		AdaBoost	0.980000019073486
	0	weka.8	SMO(1.53.2	.2)		SVM	0.97333300113678
	٢	weka.	MultiBoostA	B(1.6.2.2)		MultiBoosting	0.97333300113678
	0	weka.	Bagging(1.3	1.2.2)		Bagging	0.97333300113678
	٢	weka.	Decorate(1.	3.2.1)		Decorate	0.966666996479034
	0	weka.l	_ogitBoost(1.33)		LogitBoost	0.966666996479034
	٩	weka.F	RandomFor	est(1.6)		RandomForest	0.966666996479034
	0	weka.l	_ogistic(1.3	2)		LogisticRegression	0.959999978542328

Search: Dataset properties

OpenML	Search Share	Plugins	Developers	Community	🛔 Sign in			n <u></u> 8⁺ f
				iris Beta				
General nformation Runs	« 1 »							
	50 ¢ record	ds per page					Showing	1 to 30 of 30 entries
Data Features	Name		^ D	escription		÷	Value	▼
Data Properties	DefaultAccuracy			ne predictive accu ajority class.	uracy obtained by simply predictir	ng the	0.333333	
	EntropyClass		in ho er cl	formation needed ow 'informative' the htropy means that asses is very ske	s attribute. It determines the amound to specify the class of an instance he attributes need to be. A low cla t the distribution of examples amo wed (containing some very infrequence ne algorithms cannot handle well.	ce, or iss ong uent	1.58496	
	FeatureAbsoluteSkewness			in,max and mean ow non-normal a	s values over all features. Usually, n are calculated. Skewness is a m feature's value distribution is. Man s assume normality.	0.339639		
	FeatureAbsoluteS	skewness	m	in,max and mean	s values over all features. Usually, n are calculated. Skewness is a m feature's value distribution is. Mar	easure of	0.0189027	

Search: Quick comparisons

	OpenML	Search	Share	Plugins	Developers	Commu	inity 🌲 Sign in	1	y in Q	
Q All	Datasets	🕸 Implement	tations	I Metrics	✓ Tasks	9 Runs	Advanced	SQL	🖞 Graph	I Results

Search run results

Compare the results of multiple implementations run on multiple datasets. Results are shown in the results tab, queries can be edited in the SQL tab.

Task type

Supervised Classification

Implementations

SVM, C4.5,

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

Datasets

Collection:uci,

A comma separated list of datasets. Leave empty to include all datasets.

1. Advanced options

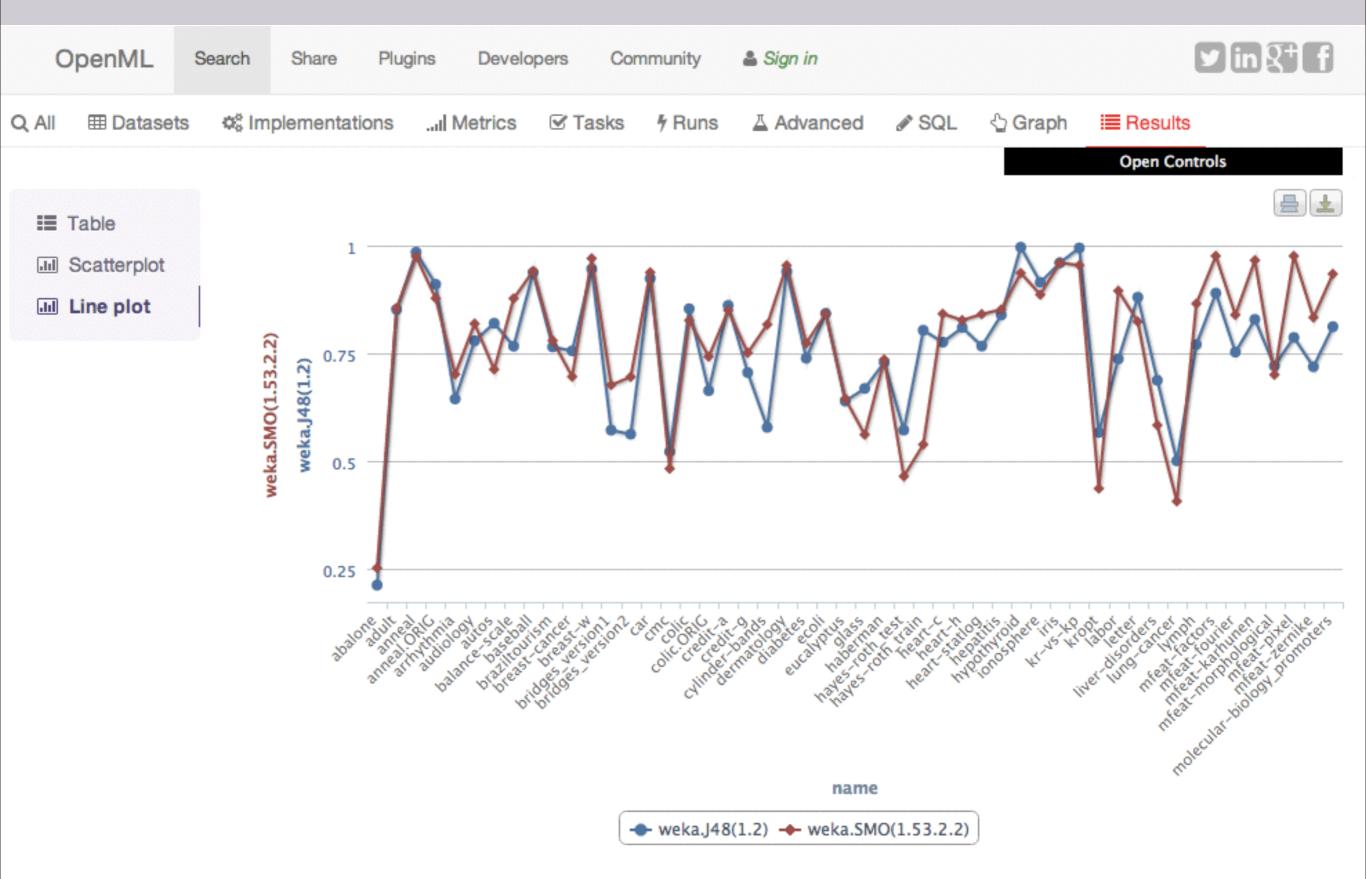
*

Run Query

Search: Quick comparisons

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I≣ Table	« 1 2 »	Crosstabulat	MyFile.csv Export -
Scatterplot	50 + records per page		Showing 1 to 50 of 87 entrie
Line plot	name	weka.J48(1.2)	weka.SMO(1.53.2.2)
	abalone	0.211634993553162	0.251376986503601
	adult	0.851705014705658	0.854367017745972
	anneal	0.984409987926483	0.974388003349304
	anneal.ORIG	0.909799993038177	0.877506017684936
	arrhythmia	0.643805027008057	0.70132702589035
	audiology	0.778761029243469	0.818584024906158
	autos	0.819512009620667	0.712194979190826
	balance-scale	0.76639997959137	0.876800000667572
	baseball	0.93731302022934	0.941044986248016
	braziltourism	0.764563024044037	0.779125988483429
	breast-cancer	0.755244970321655	0.695803999900818
	breast-w	0.945636987686157	0.969956994056702
	bridges_version1	0.571429014205933	0.67619001865387
		0.504005000405050	0.005007004404004

Search: Visualizations



Search: Advanced queries

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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

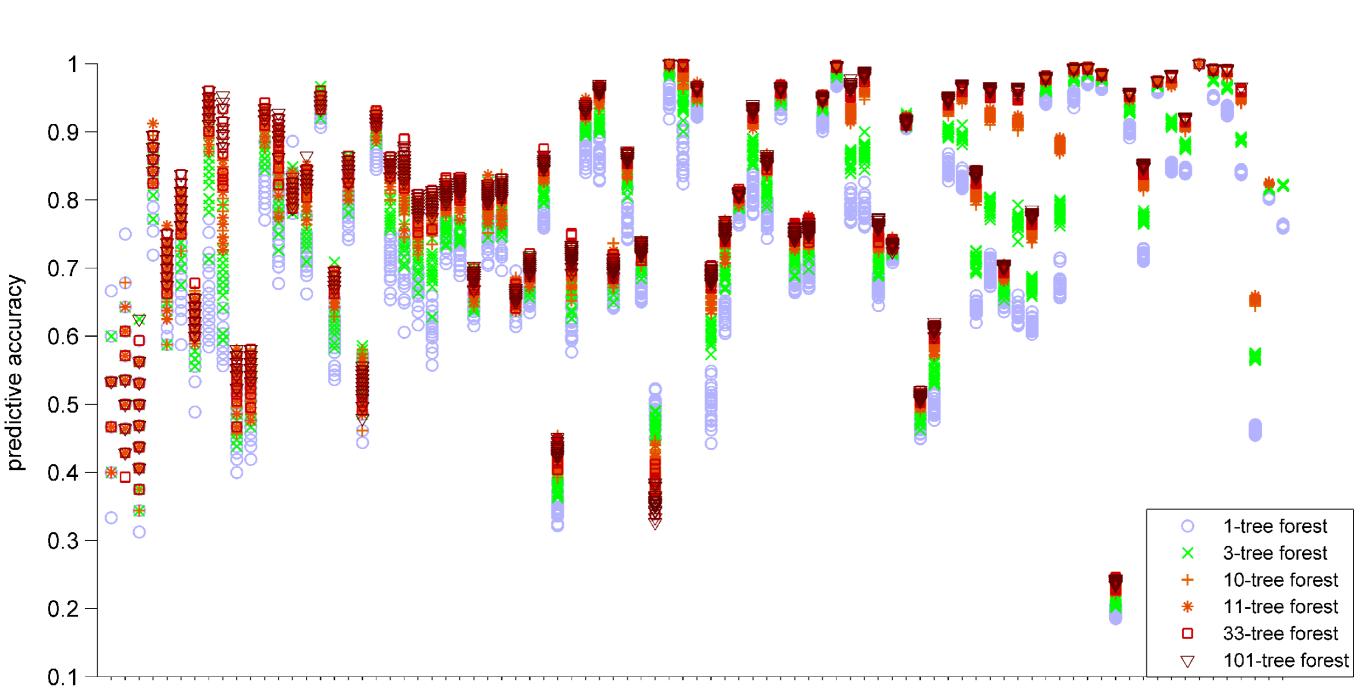
Show the effect of data property DP on the optimal value of parameter P

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

Search: Parameter effects

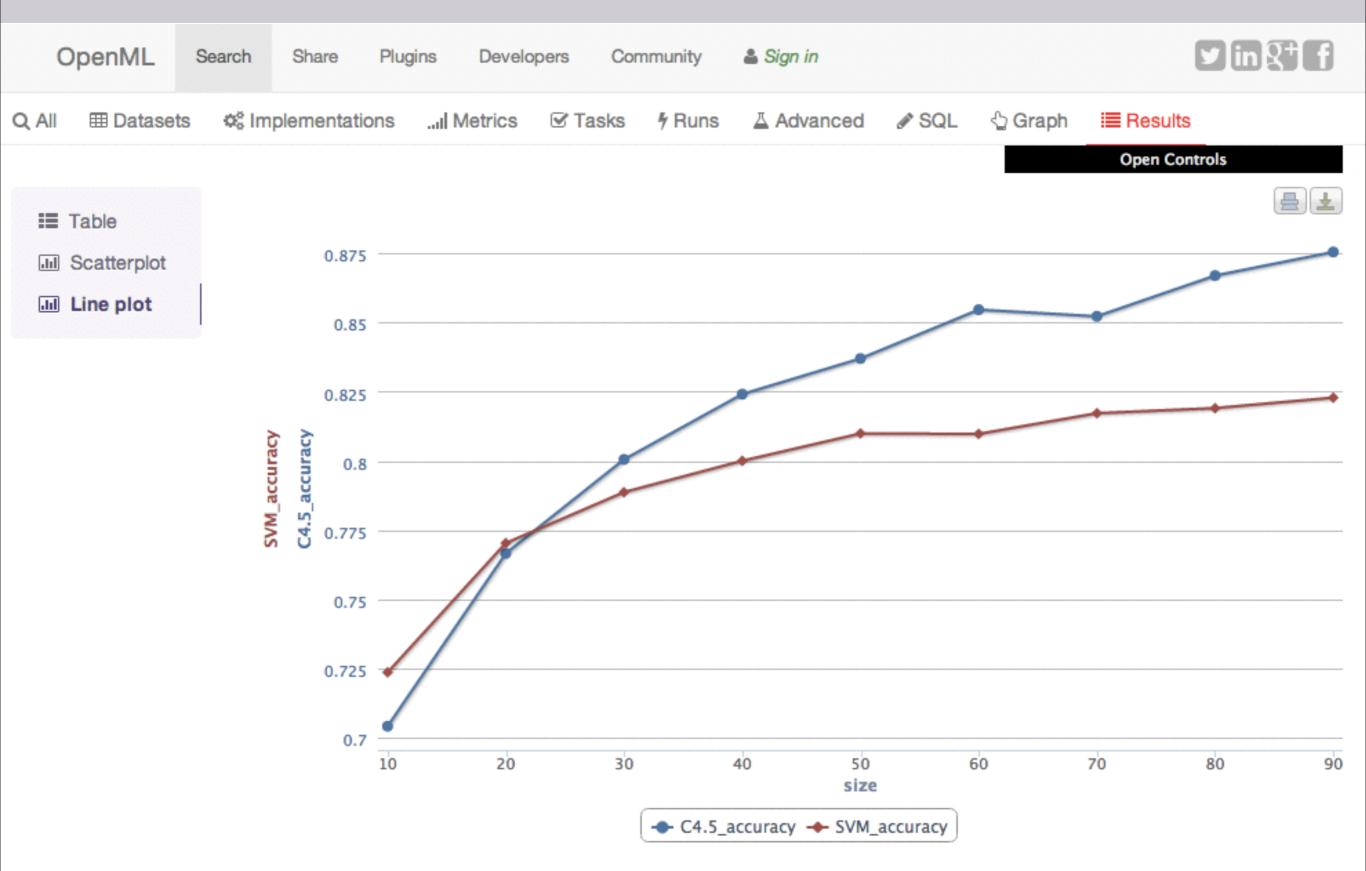


Search: Parameter effects

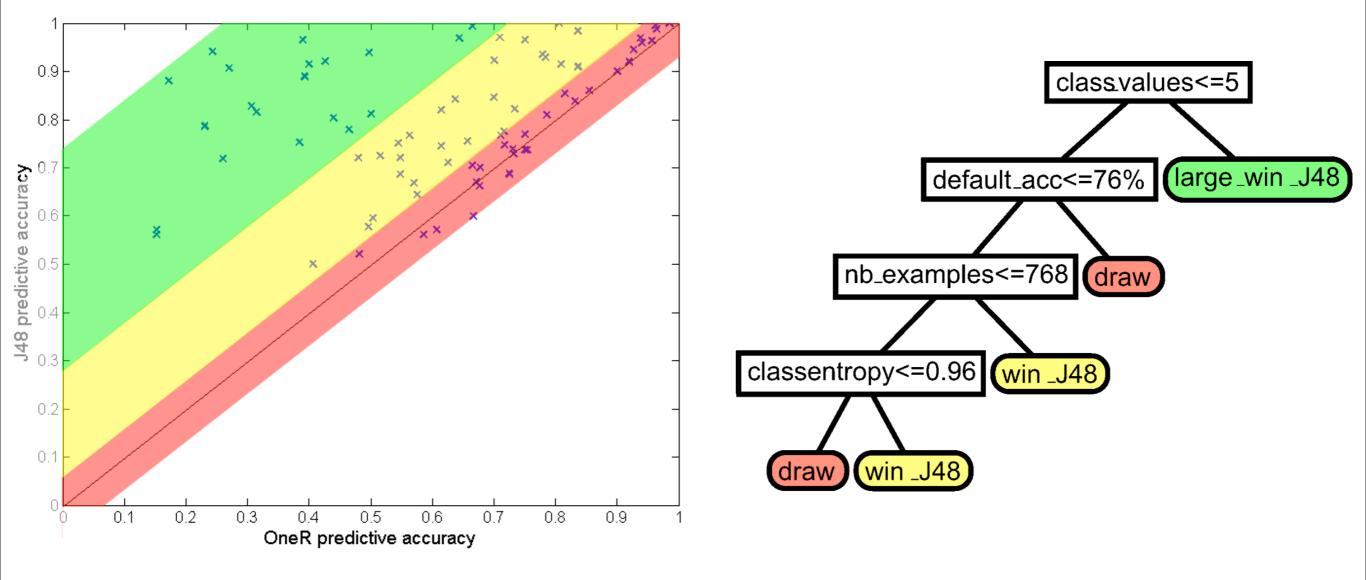


Datasets in order of increasing size

Search: Learning curves



Meta-models





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