# THE SYSTEMIC CHALLENGES OF DATA SCIENCE INITIATIVES (AND SOME SOLUTIONS)

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CNRS & University Paris Saclay



## I will not talk about science

# I will talk about management (of) (data) science

#### WHERE DOES IT COME FROM?

- My eight-year of experience interfacing between high-energy physics and data science
- Our two-year experience of running PS-CDS
- Extensive collaboration with management scientist



## DATA SCIENCE IN SCIENCE (AND INDUSTRY)

- New
- Multidisciplinary
- Disruptive

## We are in search mode

#### OUTLINE

- Intro: data science, the PS-CDS
- The data science ecosystem: challenges
- Some tools

#### DATA SCIENCE IN THE WORLD



INSTITUTE FOR DATA SCIENCE



## Université Paris-Saclay

## 19 founding partners







































## Université Paris-Saclay

**19** fondateurs

**60 000** étudiants

6 000 doctorants

**15 000** étudiants en master

**8** Schools

11 000 chercheurs et enseignants-chercheurs

**300** laboratoires

8 000 publications /an

15 % de la recherche publique française

10 départements

+ horizontal multi-disciplinary and multi-partner initiatives to create cohesion







A multi-disciplinary initiative to define, structure, and manage the data science ecosystem at the Université Paris-Saclay

http://www.datascience-paris-saclay.fr/

250 researchers in 35 laboratories

#### **Biology & bioinformatics**

IBISC/UEvry LRI/UPSud Hepatinov CESP/UPSud-UVSO-Inserm IGM-I2BC/UPSud MIA/Agro MIAj-MIG/INRA LMAS/Centrale

#### Chemistry

EA4041/UPSud **Earth sciences** 

#### LATMOS/UVSQ GEOPS/UPSud IPSL/UVSO

LSCE/UVSQ LMD/Polytechnique

#### **Economy**

LM/ENSAE RITM/UPSud LFA/ENSAE

#### Neuroscience

UNICOG/Inserm U1000/Inserm NeuroSpin/CEA

#### **Particle physics** astrophysics &

cosmology LPP/Polytechnique DMPH/ONERA CosmoStat/CEA IAS/UPSud AIM/CEA LAL/UPSud

#### **Machine learning** LRI/UPSud

LTCI/Telecom CMLA/Cachan LS/ENSAE LIX/Polytechnique MIA/Agro CMA/Polytechnique LSS/Supélec CVN/Centrale LMAS/Centrale DTIM/ONERA IBISC/UEvry LIST/CEA

#### Visualization

INRIA LIMSI

#### Signal processing

LTCI/Telecom CMA/Polytechnique CVN/Centrale LSS/Supélec CMLA/Cachan LIMSI DTIM/ONERA

#### **Statistics**

LMO/UPSud LS/ENSAE LSS/Supélec CMA/Polytechnique LMAS/Centrale MIA/AgroParisTech



#### DATA SCIENCE

Design of automated methods

to analyze massive and complex data

to extract useful information



### CENTER FOR DATA SCIENCE



#### DATA CENTER

We are focusing on inference:

data → knowledge

Interfacing with HPC, cloud, storage, production, privacy, security



### WHAT IS NEW?

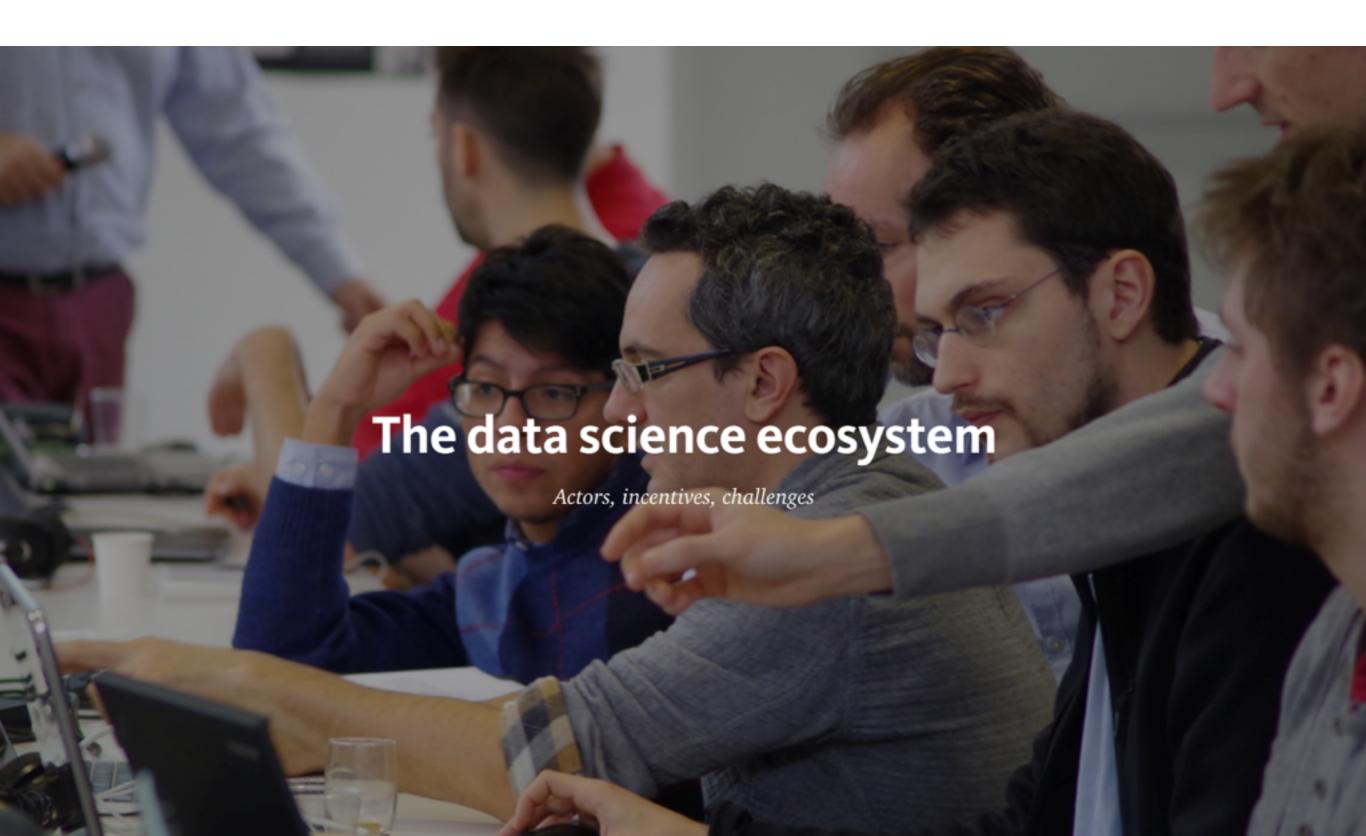
"As the flow of data increases, it is increasingly processed, analyzed, and acted upon by machines, not humans."

**NYU-CDS** manifesto

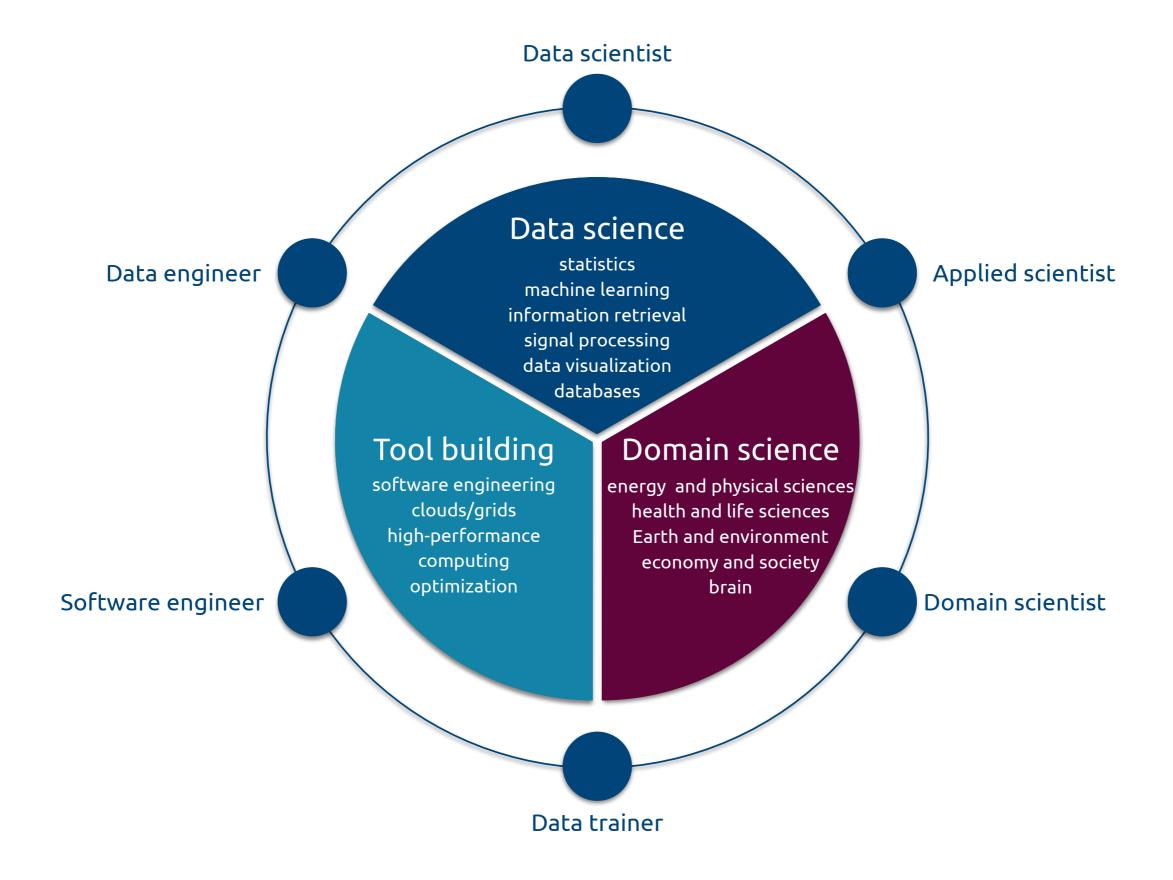
#### WHAT IS NEW?

- We have the data
  - statistical / physical modeling is less important
  - data-driven prediction
- We have the computational power
- We have the algorithms
  - · deep learning breakthrough: image, speech, language
  - closing on Al, step by step

## https://medium.com/@balazskegl



#### THE DATA SCIENCE LANDSCAPE



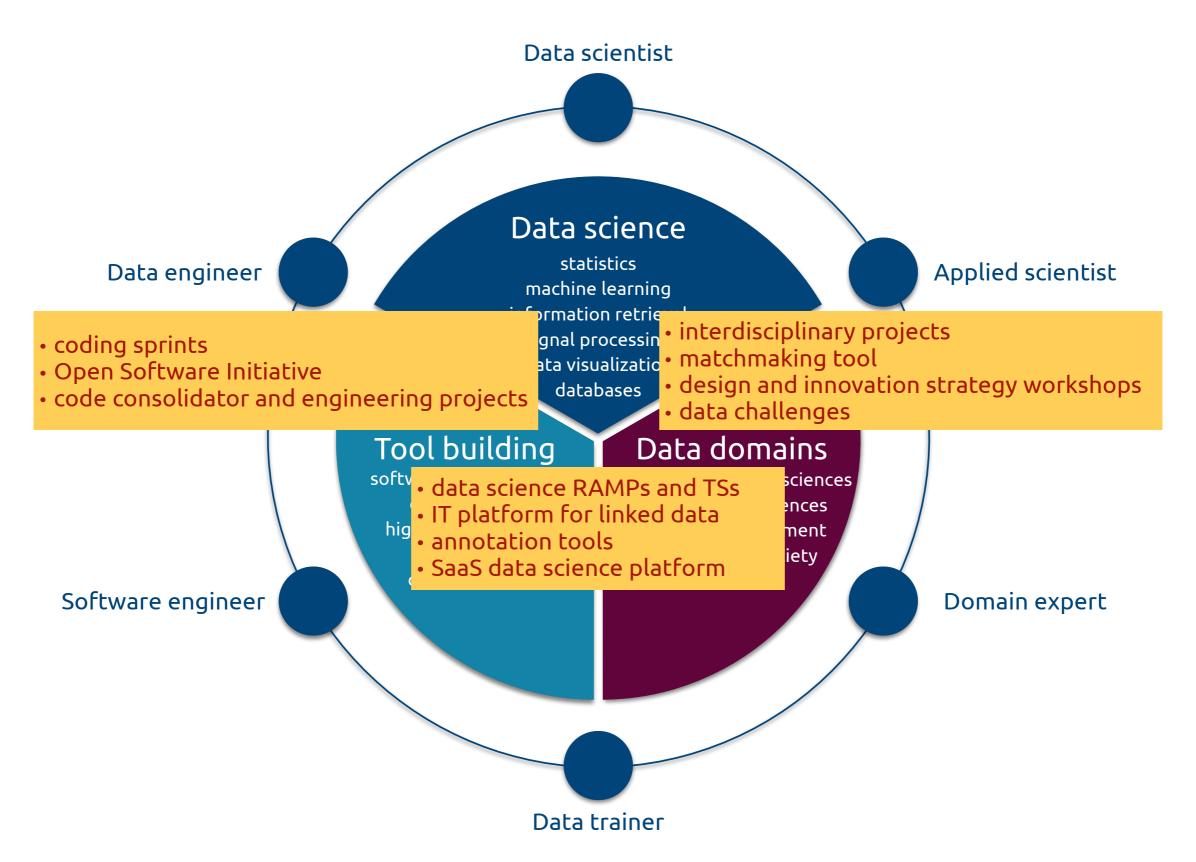
#### **CHALLENGES**

- (The lack of) manpower
  - especially at the interfaces
  - industrial brain-drain
- Incentives
  - data scientists are not incentivized to work on domain science
  - scientists are not incentivized to work on tools
- Access
  - no well-developed channels to identify the right experts for a given problem
- Tools
  - few tools that can help domain scientists and data scientists to collaborate efficiently

#### TOOLS

We are designing and learning to manage tools to accompany data science projects with different needs

#### TOOLS: LANDSCAPE TO ECOSYSTEM



## DESIGNING DATA SCIENCE PROJECTS



## DESIGNING DATA SCIENCE PROJECTS

#### Data value

#### Exploration of value

- design theory
- data-based prospection
- innovation workshops

#### Data analytics

Problem formulation Problem solving

- specialized teams
- RAMPs / training sprints
- data challenges



#### DESIGN AND INNOVATION STRATEGY WORKSHOPS

- Putting domain scientists, data scientists, and management scientist in the same room
- Getting them understand each other
- Keeping them collectively creative
- The goal: identifying and defining projects
  - low-hanging fruits
  - breakthrough projects
  - long-term vision



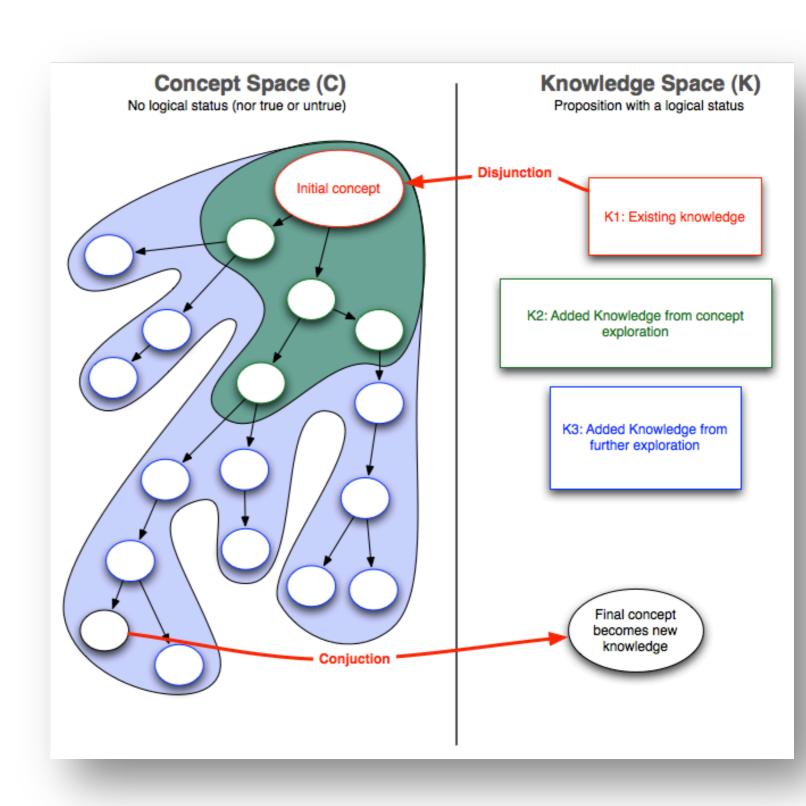
#### DESIGN AND INNOVATION STRATEGY WORKSHOPS

#### C/K design theory

innovative design

\_

interaction and joint expansion of concepts and knowledge



#### DESIGN AND INNOVATION STRATEGY WORKSHOPS

## DKCP process: linearizing C-K dynamics

Initialisation

[K] Knowledge sharing Workshops

[C] IFM-Design Workshops

[P] Project building

[RUN]





## THREE ANALYTICS TOOLS FOR DOMAIN-DATA SCIENCE INTERACTIONS

#### **DATA CHALLENGES**

RAPID ANALYTICS AND MODEL PROTOTYPING (RAMP)

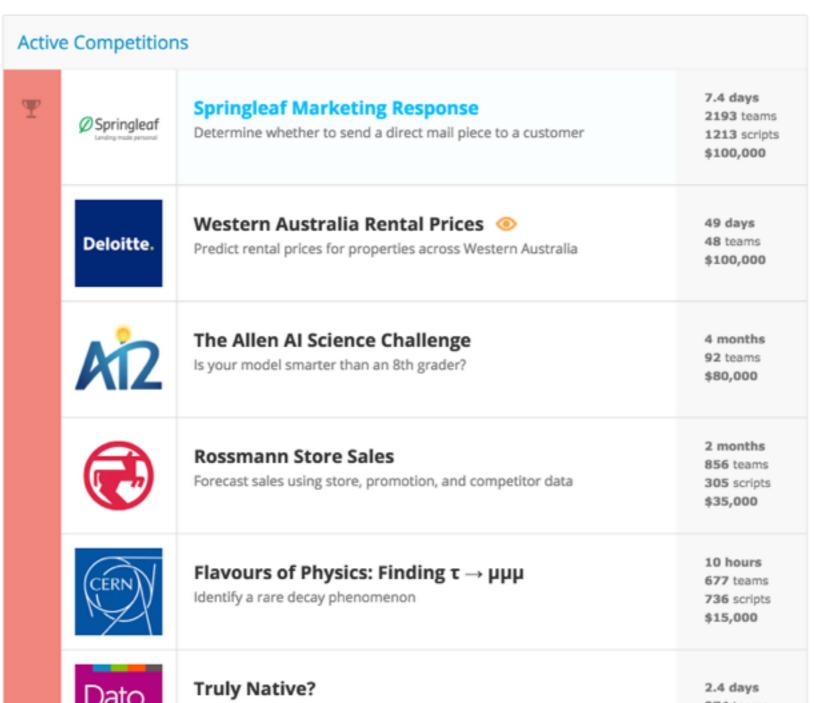
TRAINING SPRINTS (TS)



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Balazs Kegl View / Edit Profile



Is your company hiring? Are you on the job market? Visit our jobs board >>

#### Recent Jobs

AWOK.com - Senior Data Scientist (Big Data) (Dubai - UAE, Bengaluru -India)

Zynga - Senior Product Manager, Data Science (San Francisco)

DataRobot - Data Scientist (Japan)

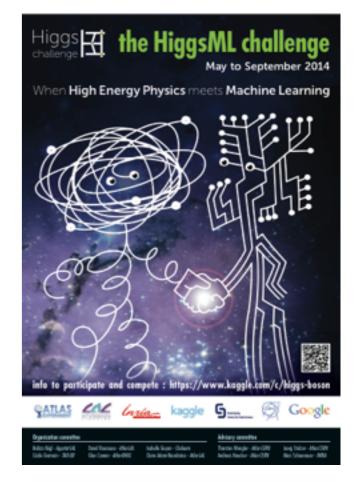
trivago - Data Scientist – Amsterdam Office (Düsseldorf)

Red Ventures - Director, Data Science (Charlotte, NC)

BBC-Group - CTO - Software Engineer Machine Learning for a new business unit (Start-Up Division) (Zurich, Switzerland)

On the Forums

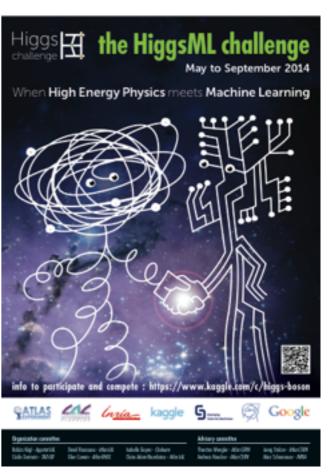
- A data challenge is a recently developed unconventional dissemination and communication tool
  - a scientific or industrial data producer arrives with a well-defined problem and a corresponding annotated data set
  - defines a quantitative goal
  - makes the problem and part of the data set (the training set) public on a dedicated site
  - data science experts then take the public training data and submit solutions (predictions) for a test set with hidden annotations
  - submissions are evaluated numerically using the quantitative measure
  - contestants are listed on a leaderboard
  - after a predefined time, typically a couple of months, the final results are revealed and the winners are awarded





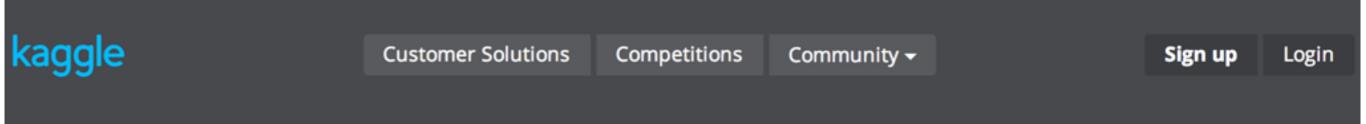


- The HiggsML challenge on Kaggle
  - https://www.kaggle.com/c/higgs-boson





## CLASSIFIAGE PUBPIC PISCOVERY





Completed • \$13,000 1,785 teams
Higgs Boson Machine Learning Challenge

Mon 12 May 2014 - Mon 15 Sep 2014 (21 days ago)

Dashboard

Private Leaderboard - Higgs Boson Machine Learning Challenge

This competition has completed. This leaderboard reflects the final standings.

See someone using multiple accounts? Let us know.

#	Δ1w	Team Name ‡model uploaded * in the money	Score ②	Entries	Last Submission UTC (Best – Last Submission)
1	<b>↑4</b>	Gábor Melis ‡ *	3.80581	110	Sun, 14 Sep 2014 09:10:04 (-0h)
2	11	Tim Salimans ‡ *	3.78913	57	Mon, 15 Sep 2014 23:49:02 (-40.6d)
3	_	nhlx5haze ‡ *	3.78682	254	Mon, 15 Sep 2014 16:50:01 (-76.3d)

## SIGNELASSIFIMATOREMENTO BYTELSTIP VERBLINE

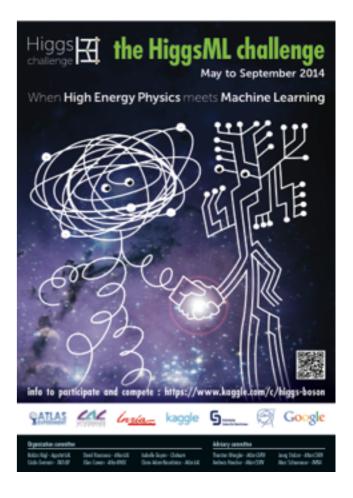
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1	<b>↑4</b>	Gábor Melis ‡ *	3.80581 1	Sun, 14 Sep 2014 09:10:04 (-0h)
2	Į1	Tim Salimans ‡ *	57	7 Mon, 15 Sep 2014 23:49:02 (-40.6d)
3	_	nhlx5haze ‡ *	3.78682 25	4 Mon, 15 Sep 2014 16:50:01 (-76.3d)
4	<b>↑55</b>	ChoKo Team 🖺	3.77526 21	6 Mon, 15 Sep 2014 15:21:36 (-42.1h)
5	<b>↑23</b>	cheng chen	3.77384 21	Mon, 15 Sep 2014 23:29:29 (-0h)
6	<b>↓2</b>	quantify	3.77086 8	Mon, 15 Sep 2014 16:12:48 (-7.3h)
7	<b>↑73</b>	Stanislav Semenov & Co (HSE Yandex)	3.76211 68	Mon, 15 Sep 2014 20:19:03
8	11	Luboš Motl's team 🎩	3.76050 58	9 Mon, 15 Sep 2014 08:38:49 (-1.6h)
9	11	Roberto-UCIIIM	3.75864 29	2 Mon, 15 Sep 2014 23:44:42 (-44d)
10	<b>↑5</b>	Davut & Josef 🎩	3.75838 16	Mon, 15 Sep 2014 23:24:32 (-4.5d)
990	<b>165</b>	sandy	3.20546 5	Fri, 29 Aug 2014 18:14:30 (-0.7h)
991	165	Rem.	2	Mon, 16 Jun 2014 21:53:43 (-30.4h)
•		simple TMVA boosted trees	3.19956	
992	<b>165</b>	Xiaohu SUN	3	Tue, 03 Jun 2014 13:14:47
993	<b>165</b>	Pierre Boutaud	3.19956 10	Fri, 25 Jul 2014 15:25:07 (-30d)

#### HUGE PUBLICITY

#### SIGNIFICANT IMPROVEMENT OVER THE BASELINE

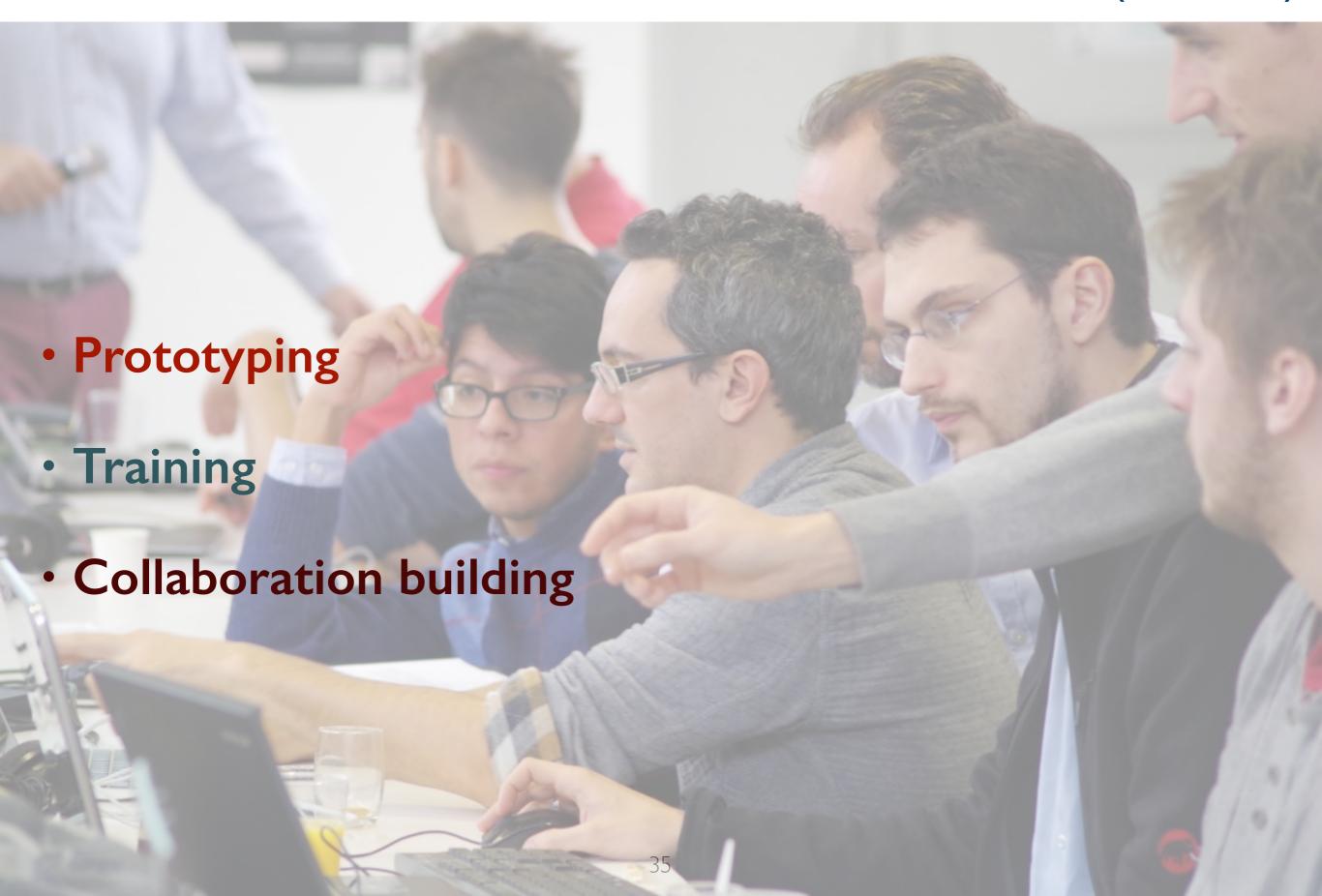
yet partially missing the objectives

- Challenges are useful for
  - generating visibility in the data science community about novel application domains
  - benchmarking in a fair way state-of-the-art techniques on well-defined problems
  - finding talented data scientists
- Limitations
  - not necessary adapted to solving complex and open-ended data science problems in realistic environments
  - no direct access to solutions and data scientist
  - emphasizes competition



We decided to design something better

#### RAPID ANALYTICS AND MODEL PROTOTYPING (RAMP)



#### **RAMPs**

- Single-day coding sessions
  - 20-40 participants
  - preparation is similar to challenges
- Goals
  - focusing and motivating top talents
  - promoting collaboration, speed, and efficiency
  - solving (prototyping) real problems



## TRAINING SPRINTS

- Single-day training sessions
  - 20-40 participants
  - focusing on a single subject (deep learning, model tuning, functional data, etc.)
  - preparing RAMPs

## ANALYTICS TOOLS TO PROMOTE COLLABORATION AND CODE REUSE



#### El Nino prediction

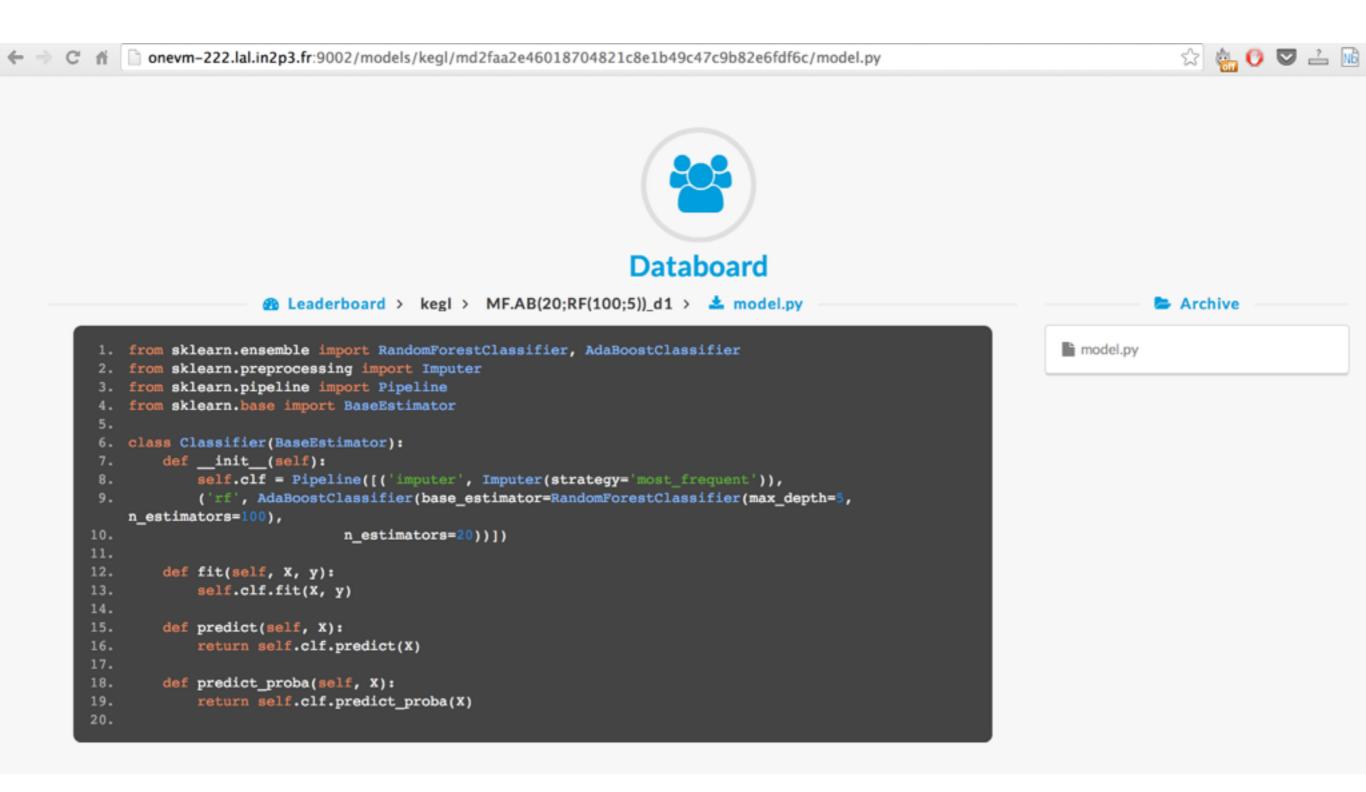
#### Leaderboard

rank	team	model	commit	score -	contributivity	train time	test time
1	CloudySunset	more_samples	2015-09-26 22:46:36	0.4336	6	95	0
2	slay	oceanmask	2015-09-26 22:46:52	0.4377	1	26	3
3	slay	grd_gbrs	2015-09-26 21:47:10	0.4390	0	30	3
4	ChrisFarley	gbr_1	2015-09-26 22:41:37	0.4390	0	30	3
5	slay	alleqlags	2015-09-26 22:48:12	0.4437	0	64	24
6	slay	detrend	2015-09-26 22:50:58	0.4437	0	66	26
7	slay_new	simplified	2015-09-26 23:43:47	0.4437	0	74	28
8	CloudySunset	tdiff_box	2015-09-26 22:21:24	0.4450	13	19	0
9	VESP	kernel-pca-elastic-net	2015-09-26 22:28:20	0.4480	11	20	2
10	slay	grd_gbr	2015-09-26 21:42:13	0.4520	0	21	3
11	CloudySunset	sd_fix_2	2015-09-26 23:59:55	0.4537	0	108	2
12	VESP	kernel-pca-linear-regression	2015-09-26 22:22:38	0.4550	1	24	2
13	VESP	kernel-pca-sea-mask	2015-09-26 22:24:27	0.4555	3	23	2
14	Earth	hyper	2015-09-27 08:58:40	0.4583	0	67	2
15	CloudySunset	more_short	2015-09-26 21:34:30	0.4653	0	17	0
16	slay	lagtemps_gbr	2015-09-26 21:15:25	0.4723	0	14	2

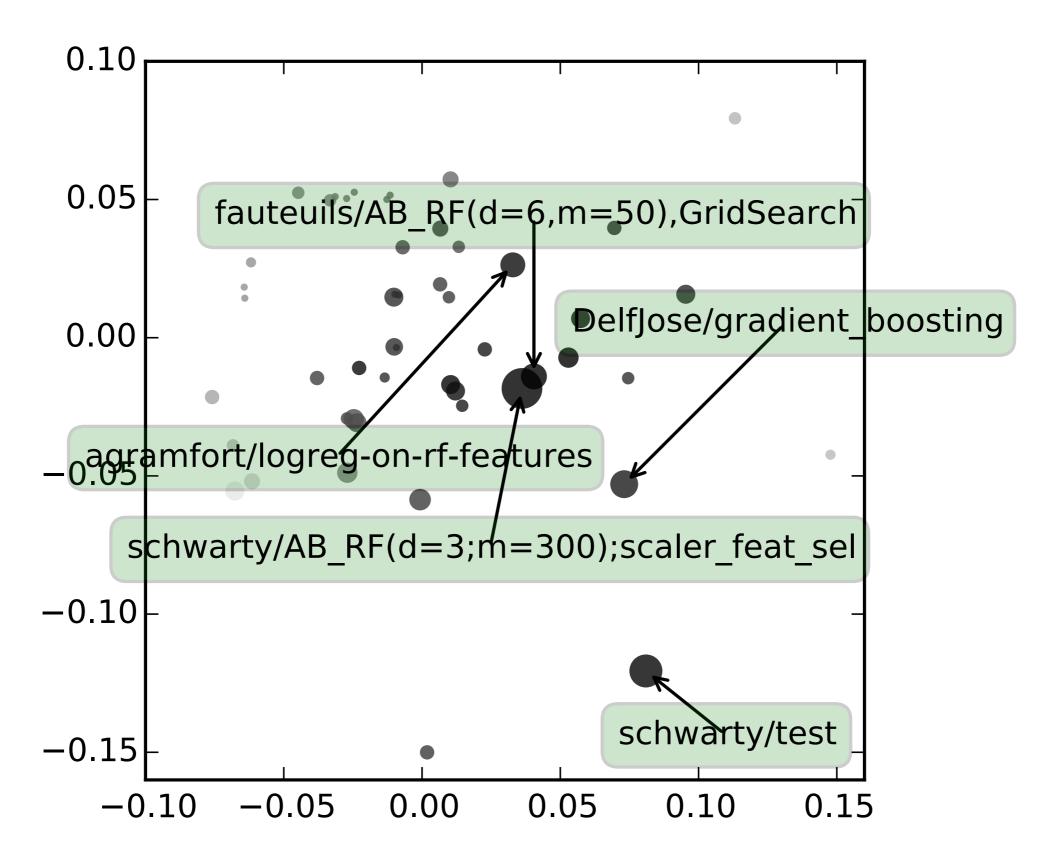
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9	<b>11</b>	Roberto-UCIIIM	3.75864	292	Mon, 15 Sep 2014 23:44:42 (-44d)
10	<b>↑5</b>	Davut & Josef 🎩	3.75838	161	Mon, 15 Sep 2014 23:24:32 (-4.5d)
990	<b>‡65</b>	sandy	3.20546	5	Fri, 29 Aug 2014 18:14:30 (-0.7h)
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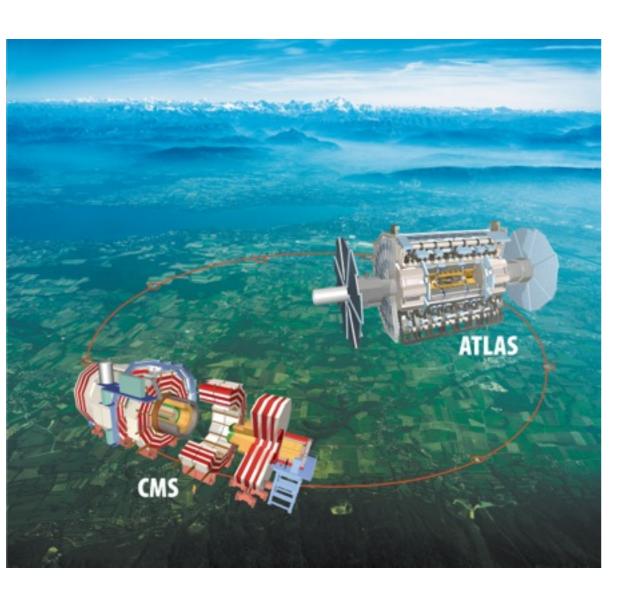
## ANALYTICS TOOL TO PROMOTE COLLABORATION AND CODE REUSE

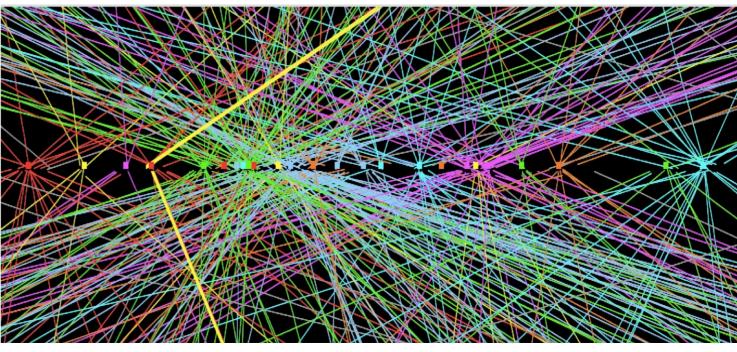


## **ANALYTICS TOOLS TO MONITOR PROGRESS**

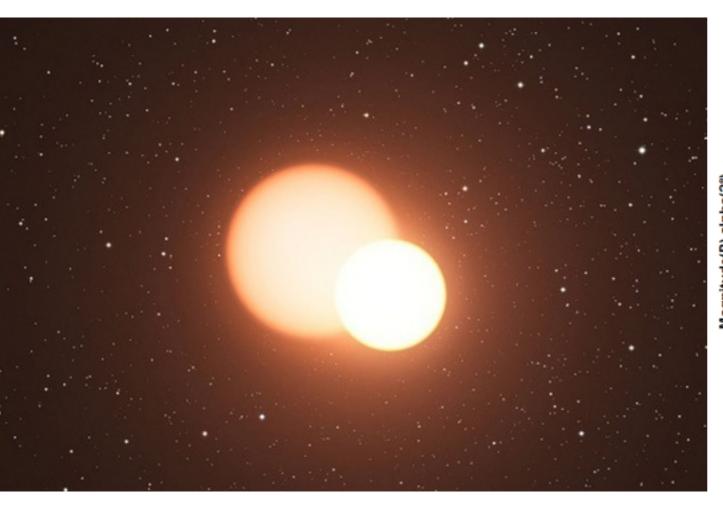


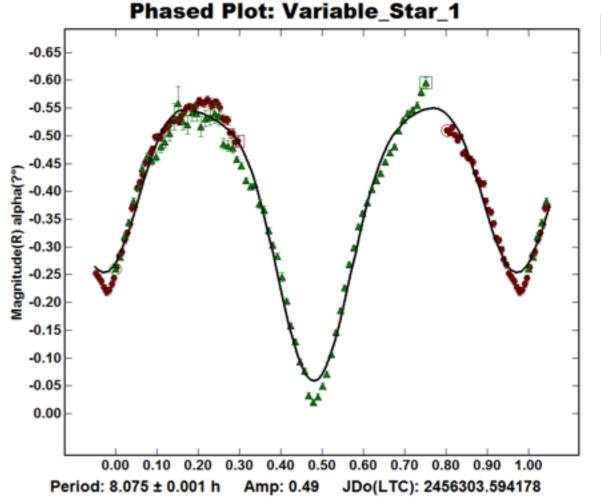
# RAPID ANALYTICS AND MODEL PROTOTYPING 2015 Jan 15 The HiggsML challenge



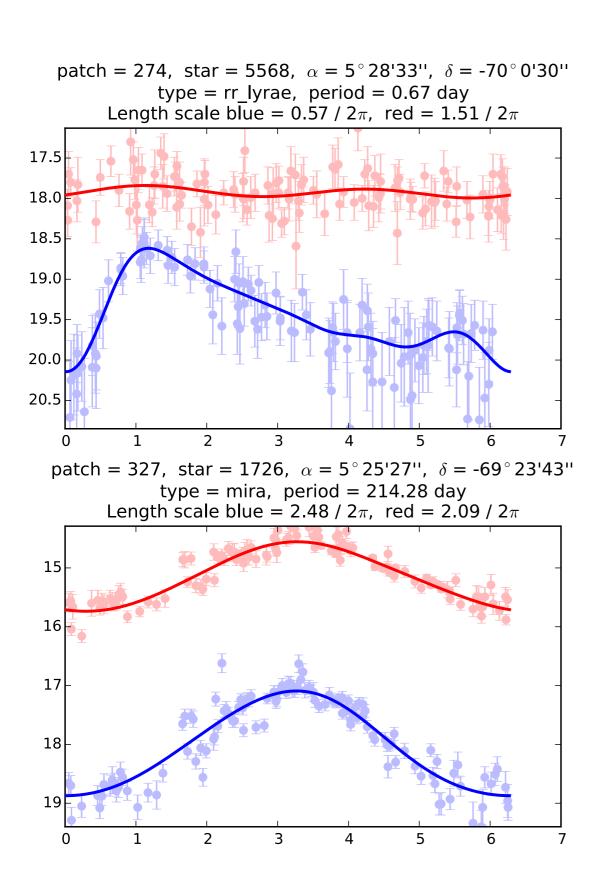


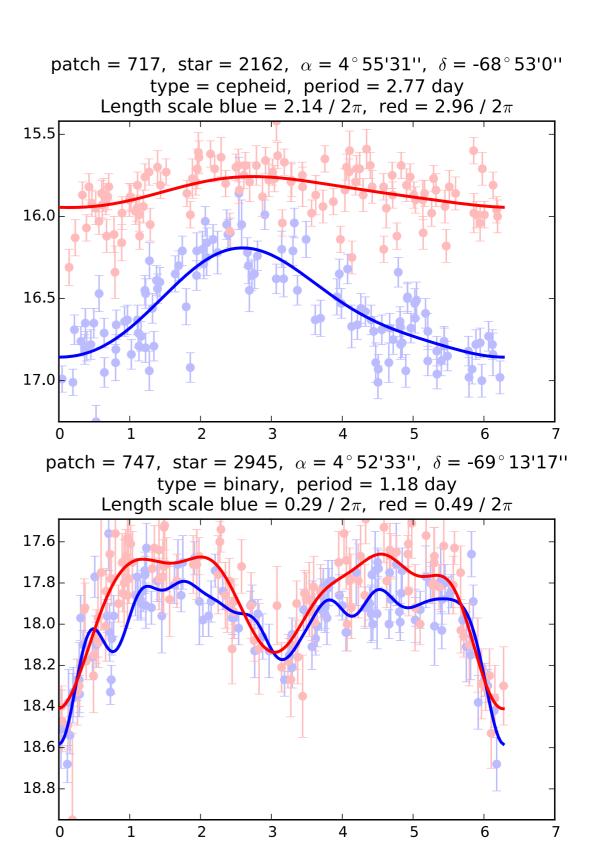
## 2015 Apr 10 Classifying variable stars





## VARIABLE STARS





## VARIABLE STARS



Variable star type prediction

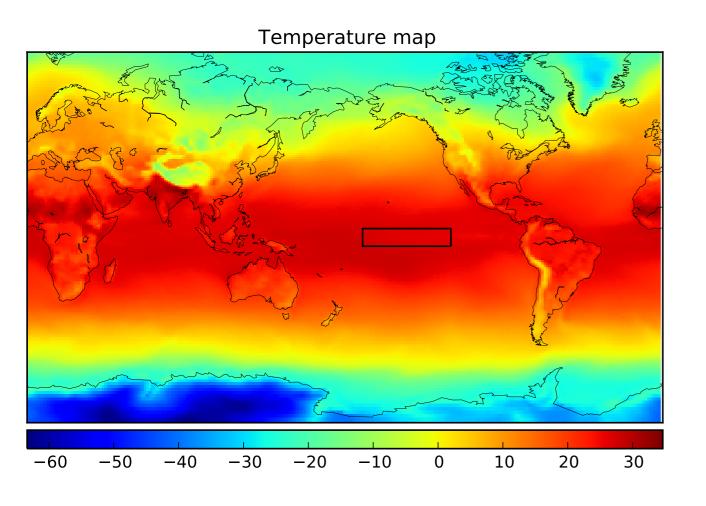
#### Leaderboard

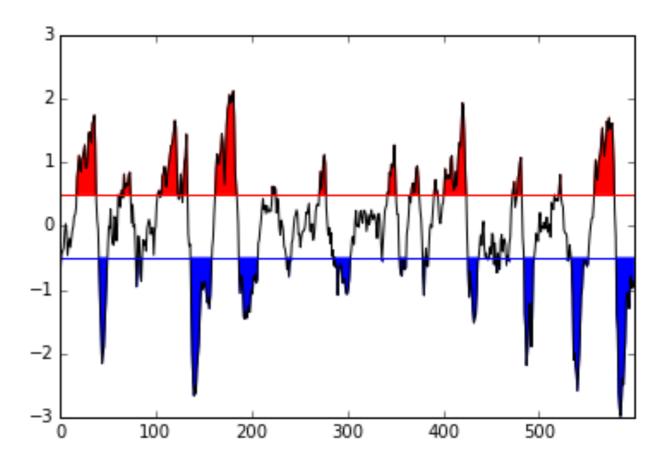
rank	team	model	commit	score 🔺	contributivity	train time	test time
1	LesTortuesNinja	gp_fixed_3	2015-04-11 00:48:59	0.9621	19	117	103
2	agramfort	gp_rf30_adaboost10_v2	2015-04-10 14:30:50	0.9596	3	117	104
3	Overfitters	stack_wavelet	2015-04-10 17:03:27	0.9588	6	313	132
	A1 171		2045 04 40 47 40 00	0.0500	_	4.40	400

## accuracy improvement: 89% to 96%

		— — — — — — — — — — — — — — — — — — —					
7	delphine	feature_selection	2015-04-10 14:46:38	0.9577	4	117	109
8	delphine	first_test	2015-04-10 13:18:41	0.9574	1	127	110
9	bekou	fifthattempt	2015-04-10 17:33:31	0.9563	2	134	114
10	agramfort	gp_rf_adaboost_v3_gp_fix	2015-04-10 17:30:16	0.9555	1	93	84
11	anon	try_04_ab_gbc	2015-04-10 18:01:31	0.9552	2	149	101
12	bekou	firstmodel	2015-04-10 13:56:21	0.9550	4	146	116
13	2AN	eleventh	2015-04-10 16:40:54	0.9544	0	123	106
14	2AN	nineth	2015-04-10 16:38:22	0.9544	3	119	112
15	2AN	twelve	2015-04-10 16:40:54	0.9544	0	124	108
16	LesTortuesNinja	gp_2	2015-04-09 10:53:57	0.9544	0	134	117
17	Madclam	second_try_w_gp	2015-04-10 13:11:38	0.9544	0	136	111
40	0(!!!	in the state of the state of	2045 04 40 40 44 04	0.0544		404	400

## 2015 June 16 and Sept 26 Predicting El Nino









#### El Nino prediction

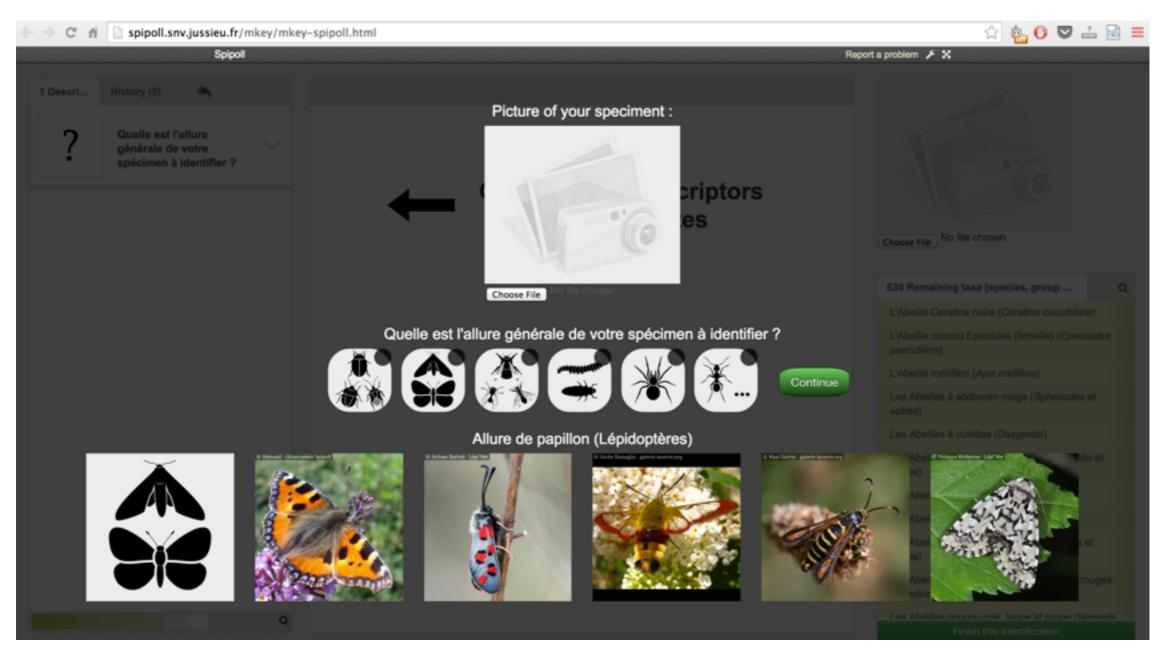
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2	slay	oceanmask	2015-09-26 22:46:52	0.4377	1	26	3
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4	ChrisFarley	gbr_1	2015-09-26 22:41:37	0.4390	0	30	3

## RMSE improvement: 0.9°C to 0.4°C

8	CloudySunset	tdiff_box	2015-09-26 22:21:24	0.4450	13	19	0
9	VESP	kernel-pca-elastic-net	2015-09-26 22:28:20	0.4480	11	20	2
10	slay	grd_gbr	2015-09-26 21:42:13	0.4520	0	21	3
11	CloudySunset	sd_fix_2	2015-09-26 23:59:55	0.4537	0	108	2
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13	VESP	kernel-pca-sea-mask	2015-09-26 22:24:27	0.4555	3	23	2
14	Earth	hyper	2015-09-27 08:58:40	0.4583	0	67	2
15	CloudySunset	more_short	2015-09-26 21:34:30	0.4653	0	17	0
16	slay	lagtemps_gbr	2015-09-26 21:15:25	0.4723	0	14	2
17	slay	galapagos	2015-09-26 22:05:54	0.4725	0	17	2
18	CloudySunset	gbr_world_2	2015-09-26 19:3743/8	0.4756	0	11	0

## 2015 October 8 Insect classification





Pollenating insect classification

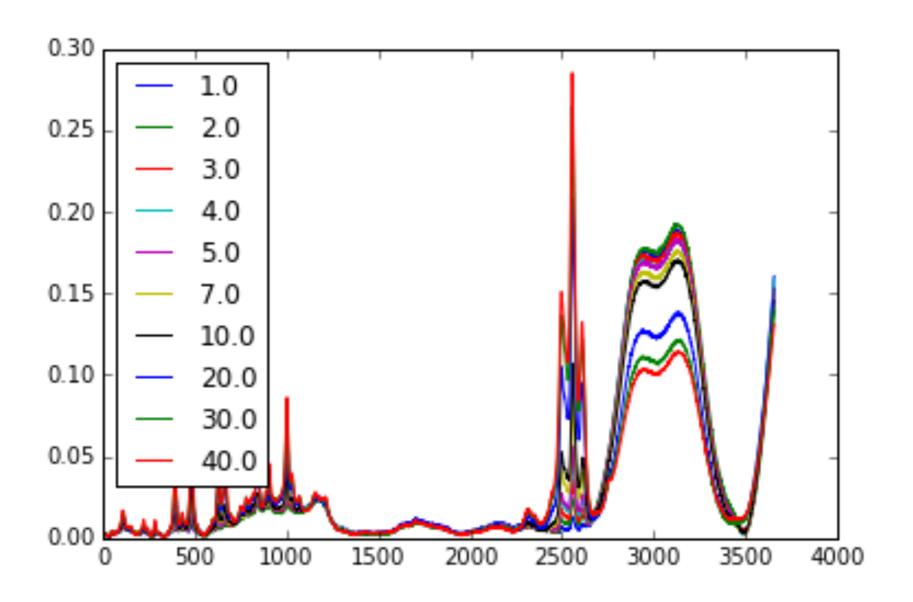
#### Leaderboard

rank	team	model	commit	score -	contributivity	train time	test time
1	Florian	yousra_with_flip_rotation_gaussian_windo[]	2015-10-08 18:11:52	0.7194	30	3735	1
2	Florian	yousra_with_flip_rotation_gaussian_windo[]	2015-10-08 17:20:19	0.6812	2	2646	1
3	Issam	rotation_noreg_yousra_first_3	2015-10-08 17:31:38	0.6801	15	1235	1
4	Brutti	small_rot_fix	2015-10-08 18:01:18	0.6654	17	3757	1

## accuracy improvement: 30% to 75%

8	Issam	rotation_regularization_yousra_first_4	2015-10-08 17:32:54	0.6577	1	1758	1
9	Brutti	small_rot	2015-10-08 17:26:27	0.6575	3	3066	1
10	Issam	rotation_regularization_yousra_first_3	2015-10-08 17:32:54	0.6531	5	1531	1
11	YousraB	yousra_yousra	2015-10-08 17:17:38	0.6461	0	609	1
12	lambdacoder	model_4	2015-10-08 16:27:11	0.6440	0	567	1
13	lambdacoder	model_5	2015-10-08 17:04:03	0.6364	0	613	1
14	wa_team	wa_round_crop	2015-10-08 17:39:35	0.6357	0	660	1
15	Florian	hedi2_flip_rotation_crop	2015-10-08 14:26:47	0.6271	0	1210	1
16	lambdacoder	model_9	2015-10-08 18:10:17	0.6245	6	1756	1
17	Tony	noisy_batch2	2015-10-08 18:01:34	0.6207	3	895	1
18	MatW	rotation_8	2015410-08 17:08:01	0.6198	0	2016	1

## 2015 Fall Drug identification from spectra



## THANK YOU!

## IT PLATFORM FOR LINKED DATA

## http://io.datascience-paris-saclay.fr/

- A window to open data at Paris-Saclay
- · We are not storing or handling existing large data sets
- Rather indexing, linking, and mapping, embedding in the worldwide linked data (RDF) ecosystem
- Storing small data sets of small teams is possible
- Subsets of large sets for prototyping
- Or simply store metadata plus pointer



## IT PLATFORM FOR LINKED DATA

