Machine learning for scientific workflows
Managing the data science process

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Who am I?

Balázs Kégl

- Senior researcher **CNRS**
  - machine learning (20+ years)
    interfacing with particle physics (10+ years)
- Head of the **Paris-Saclay Center for Data Science**
  - interfacing with biology, economy, climatology, chemistry, etc. (4 years)
  - industrial ML projects (4 years)

OUTLINE

- Machine learning for **scientific workflows**
  - **challenges**
  - **use cases**: data collection, inference, simulation
  - **examples**: pollenating insects, autism, variable stars, Mars craters, drug spectra, the Higgs boson, El Nino
- Managing the data science process: the **RAMP framework**
  - **roles** and **tasks** in the **data science process**
  - **building** the workflow: **who does what**
  - what is a **predictive workflow**, what are the **parametrizable components**
  - how to make **data scientists efficient**

Why is this relevant for you?

- Typical **ML** research project
  - take an **existing ML problem** (e.g., image classification)
  - scan **literature**
  - install/develop **experimental environment**
  - **explore ideas** to find new solutions
  - **optimize**, show they work **better than existing solutions**, ideally on established and accepted **benchmarks**
  - publish

WHY IS THIS RELEVANT FOR YOU?

- Typical **applied** research project
  - take an **existing domain-scientific or industrial problem** (e.g., galaxy deblending)
  - scan **literature**
  - install/develop **experimental environment**
  - **collect data** and **establish benchmark**
  - apply **existing ML solution**
  - optionally fine tune, explore a **small number** of alternatives
  - show that the **ML solution is better than the classical "manual" solution** on your **own benchmark**
  - publish

Both take years, typically

How to make applied projects **faster**?

How to explore a **large number of ML solutions** in a **short time**?

LONGER TERM VISION

- Put more focus on **problem formulation**
  - **detect** important applied problems
  - agree on **metrics** and **benchmarks** and **organize data collection**
  - organizationally **separate setting up benchmarks and optimizing solutions**
  - establish a **fair and possibly “third party” framework** (see ImageNet)
  - hammer the message that **formulating scientific problems into predictive workflows is valuable research**

WHY IS THIS RELEVANT FOR YOU?

- You may use it to **accelerate your own research**
- You may remember this when you **join the data science industry**

Paris-Saclay Center for Data Science

A multi-disciplinary initiative, building interfaces, matching people, helping them launching projects

345 affiliated researchers, 50 laboratories

Biology & bioinformatics
IBISC/UEvry
LRI/UPSud
Hepatinov
CESP/UPSud-UVSQ-Inserm
IGM-I2BC/UPSud
MIA/Agro
MIAj-MIG/INRA
LMAS/Centrale

Chemistry
EA4041/UPSud

Earth sciences
LATMOS/UVSQ
GEOPS/UPSud
IPSL/UVSQ
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

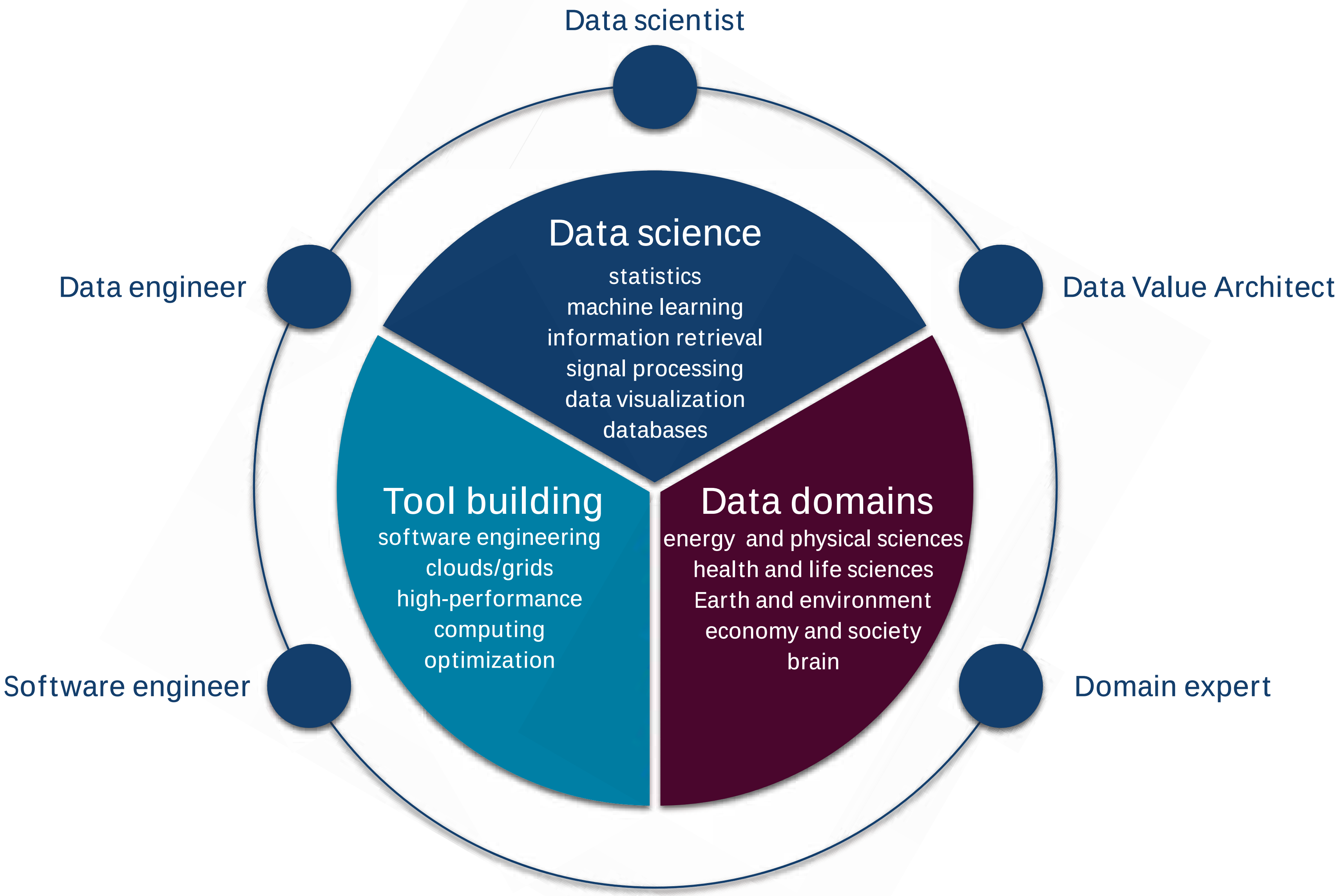
Visualization
INRIA
LIMSI

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

The data science ecosystem

https://medium.com/@balazskegl



MANAGEMENT AND ORGANIZATIONAL

- Lack of **manpower**, misplaced **incentives**
  - hammers & nails
  - engineering: who deals with production?
- Lack of **collaboration/innovation management** tools
- Bottleneck is sometimes **data collection/annotation**
  - since domain scientists do not know ML, they do not collect the *right* data

TECHNICAL CHALLENGES

- Workflows and metrics
  - Designing the **workflow**, interaction with the **rest of the pipeline**, **metrics** is often **more important than “hyperopting” the predictor**
- Data generation
  - training is often done on **simulations**, so we need to **design data generation**
  - **systematic** uncertainties
  - the **iid oracle is a fairy tale**, happening only in machine learning textbooks
  - opportunity for **diversifying ML benchmarks**

ML USE CASES IN SCIENCES

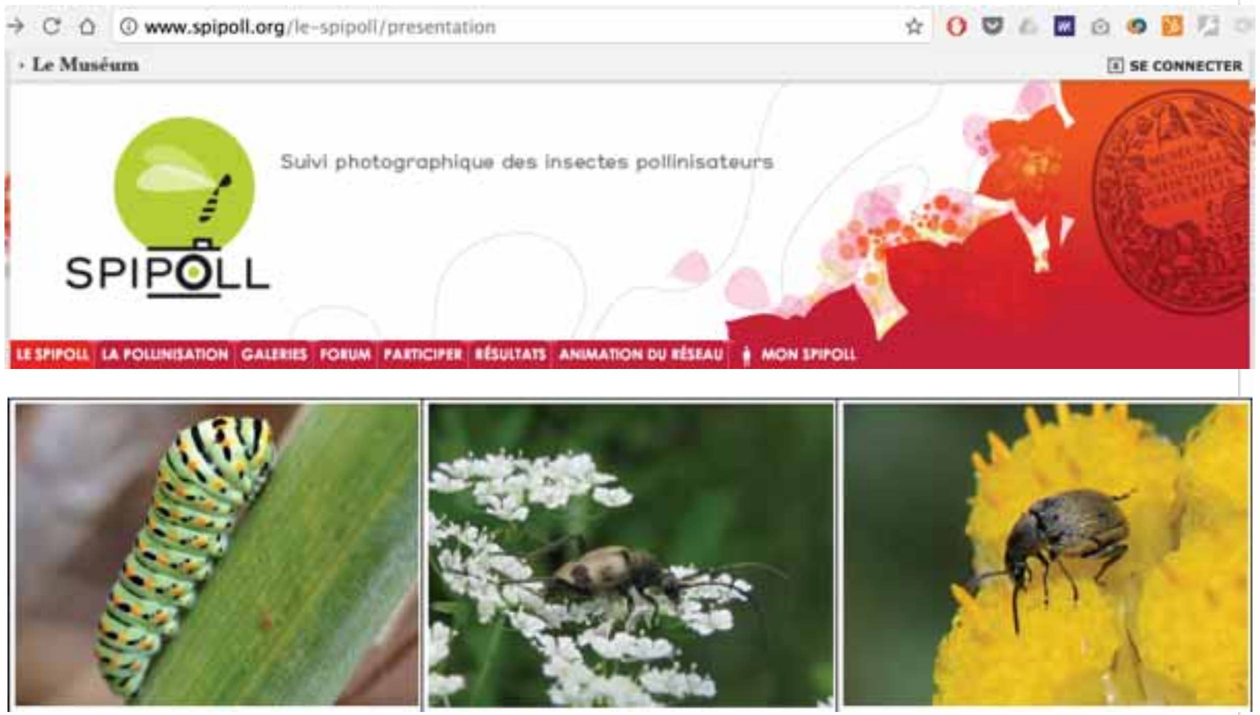
https://www.ramp.studio/problems

- **Data collection**: replace human or algorithmic collector or annotator
  - label insect photos, detect Mars craters, detect particle tracks
- **Inference**: to invert the generative model
  - "predict" a particle, detect an anomaly, **infer a parameter y from observation x**
- **Generation, model reduction**: to replace expensive simulations
  - "learn" a physics simulation or an agent based micro-economical model with a neural net
- **Hypothesis generation**: to "replace" theoreticians
  - **learn, represent structural knowledge** and **generate novelty in model space**, e.g., molecule generation in drug discovery

Data collection

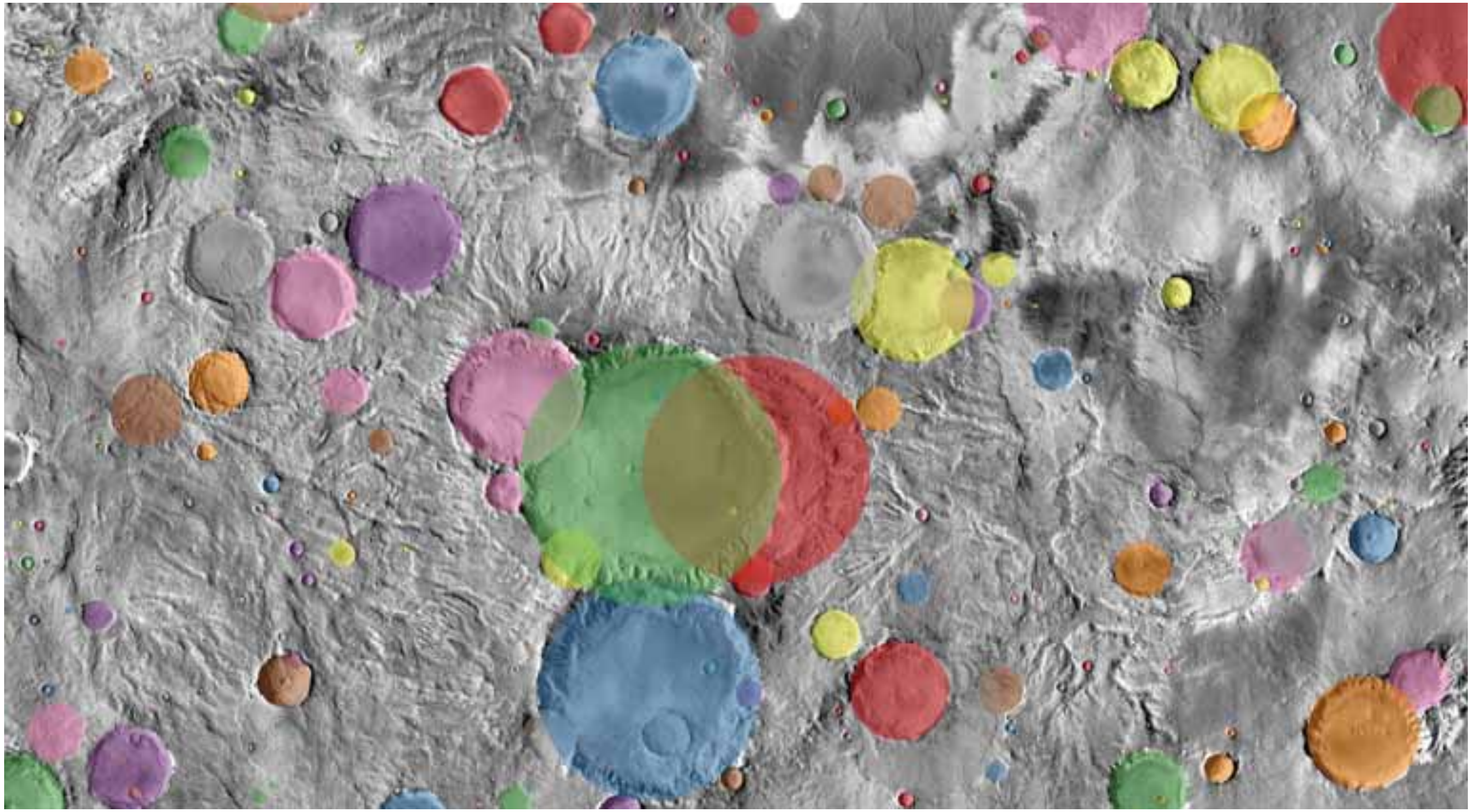
CLASSIFYING POLLENATING INSECT PHOTOS

- collaboration with **ecologists at the Paris Museum of Natural History**
- **400 classes**, **150K photos**, **long tail**
- great benchmark for **transfer** and **few-shot** learning
- developed models in **production**, powering an **android app**



DETECTING MARS CRATERS

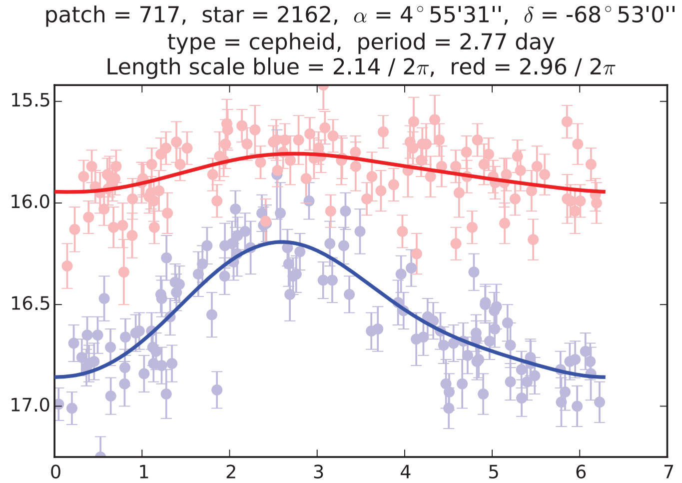
- collaboration with **planetary geologists at Paris-Saclay**
- new **metrics** and **workflow**
- great benchmark for **detection in satellite imagery**

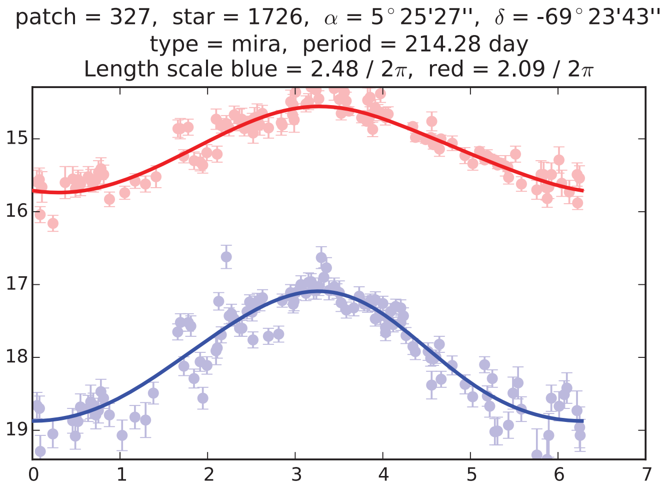


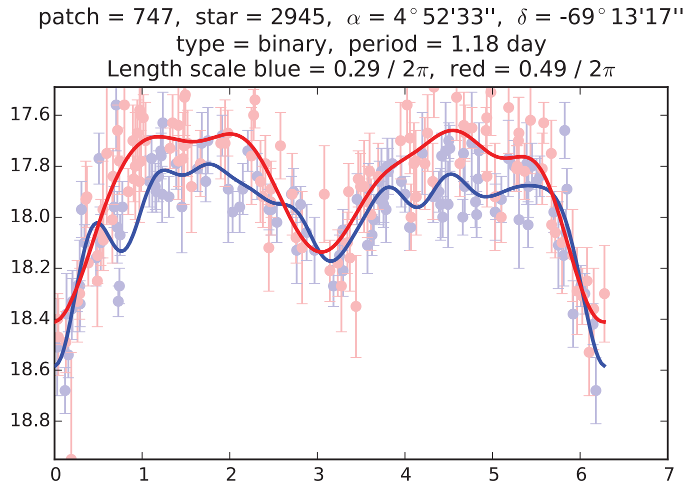
Inference

Classifying variable stars

- collaboration with **astrophysicists at Paris-Saclay**
- variable-length **functional data**



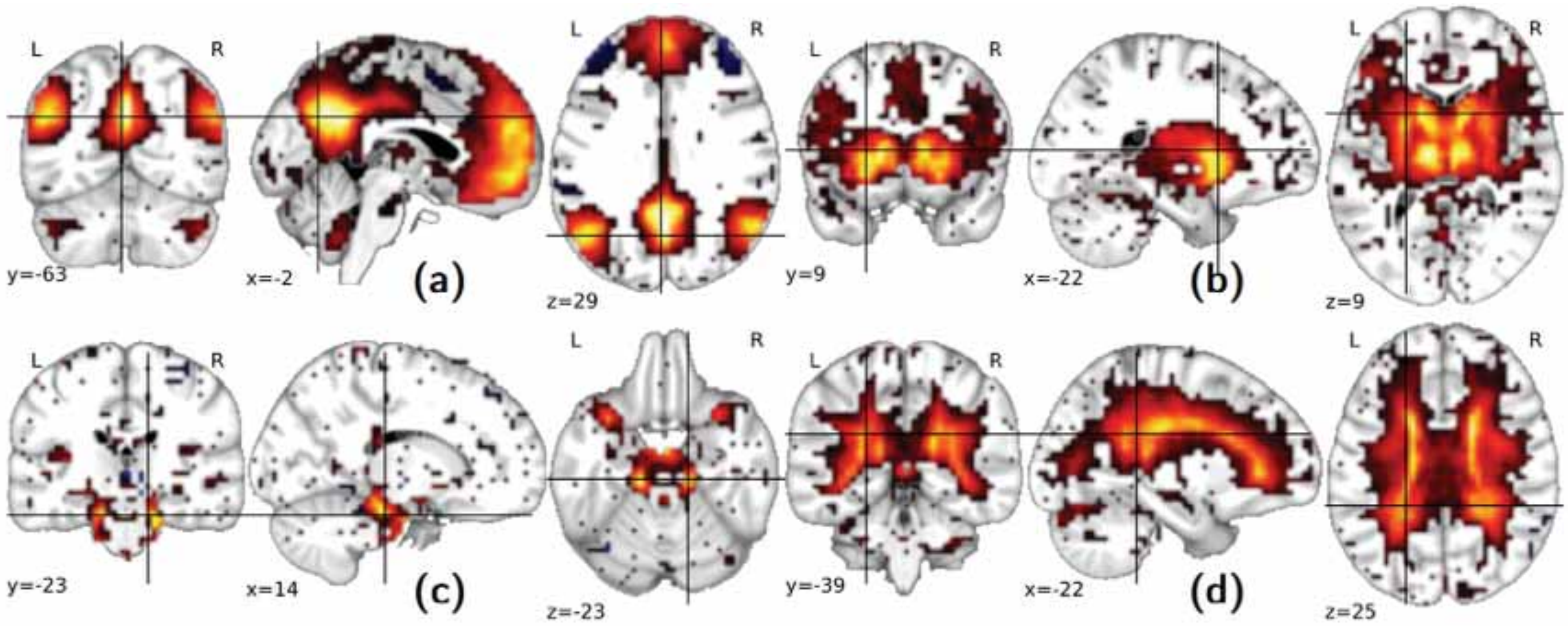




Predict autism from brain scans

https://paris-saclay-cds.github.io/autism_challenge

- collaboration with **neurologists of Institut Pasteur**
- **3000** subjects: a **major major data collection effort**
- heavy **preprocessing** and **quality control**
- **ongoing** challenge till **July 1** with **9.5K€** money prizes



CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA

- collaboration with the **pharmacy department** of Georges Pompidou Hospital
- **major data collection effort**
- functional data
- probably the first ever research paper where the **ML workflow optimization was entirely crowdsourced**

Classifying and quantifying monoclonal antibody preparations for cancer therapy using machine learning

Laetitia Le [ab], Camille Marini [ce], Alexandre Gramfort [cfg], David Nguyen [a], Mehdi Cherti [ch], Sana Tfaili [b], Ali Tfayli [b], Arlette Baillet-Guffroy [b], Eric Caudron [ab], Balázs Kégl [ch]

[a] European Georges Pompidou Hospital (AP-HP), Pharmacy department, Paris, France
[b] Lip(Sys) Chimi Analytique Pharmaceutique, Univ. Paris-Sud, Universit Paris Saclay, F92290 Chatenay-Malabry, France (EA4041 Groupe de Chimie Analytique de Paris Sud)
[c] Center of Data Science, Université Paris-Saclay
[d] Université Paris-Sud
[e] CMAP, Ecole Polytechnique, Palaiseau, France
[f] INRIA, Parietal team, Saclay, France
[g] LTCI, Télécom ParisTech
[h] LAL, CNRS, France

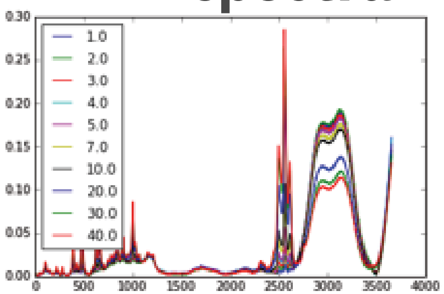
26 March 2017

CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA

chemotherapy
drug in
elastic pocket

laser
spectrometer

molecular
spectra



feature extractor 1

classifier

drug type

feature extractor 2

regressor

concentration

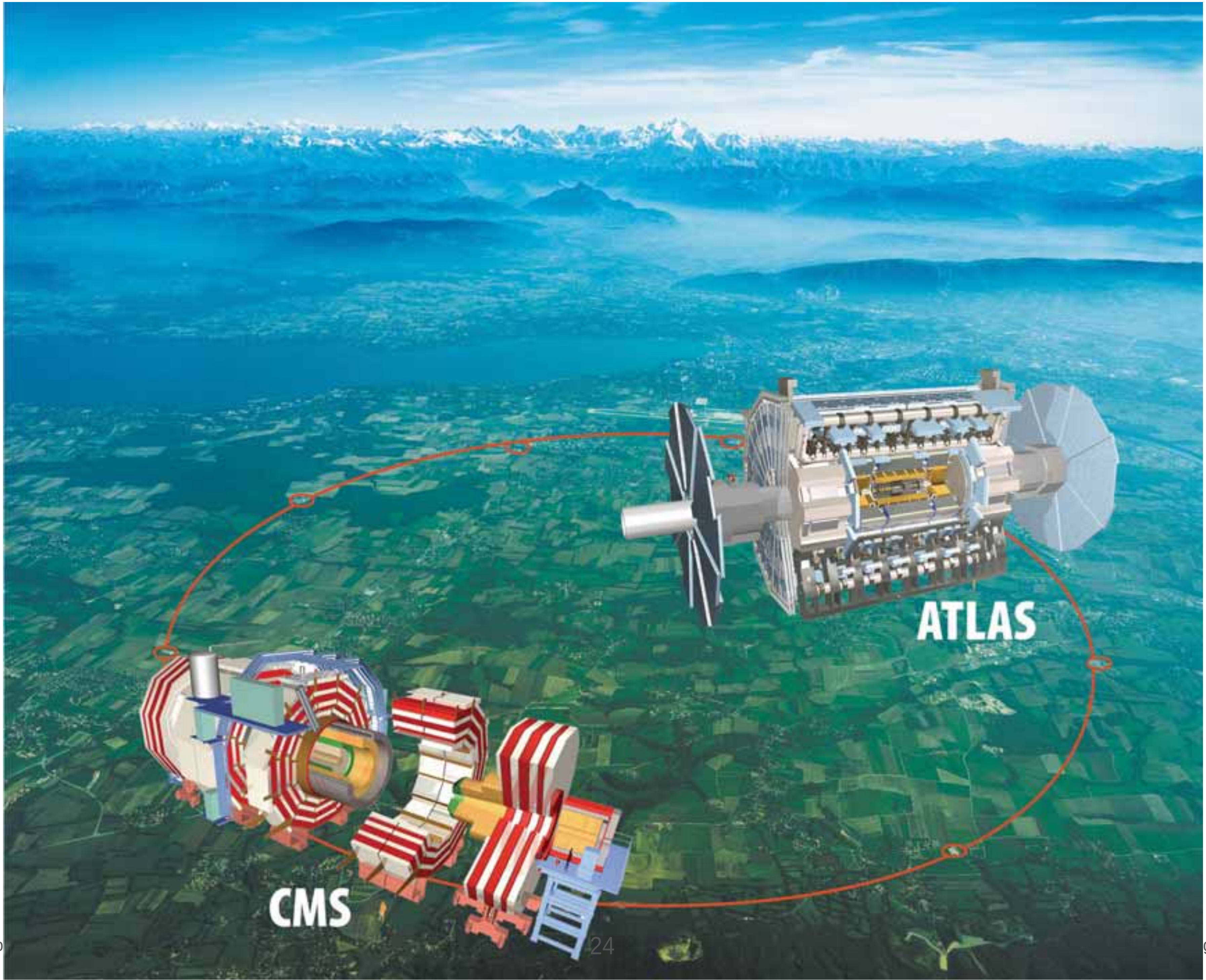
Learning to discover: the Higgs boson machine learning challenge

Claire Adam-Bourdarios[a], Glen Cowan[b], Cécile Germain[c], Isabelle Guyon[d], Balázs Kégl[a,c], David Rousseau[a]

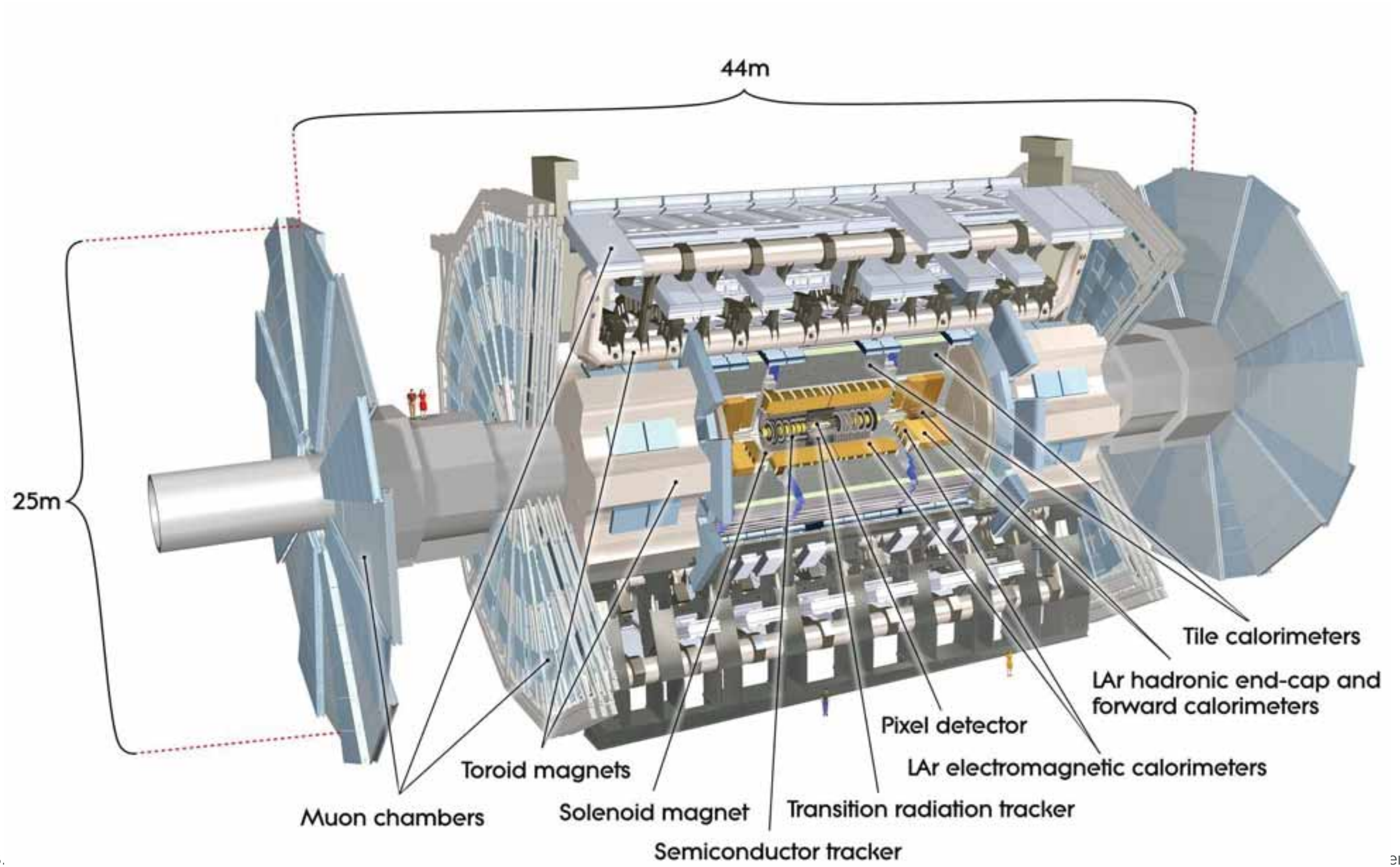
[a] LAL, IN2P3/CNRS & University Paris-Sud, France
[b] Physics Department, Royal Holloway, University of London, UK
[c] TAO team, INRIA & LRI, CNRS & University Paris-Sud, France
[d] ChaLearn

21 July 2014, version 1.8

THE LHC IN GENEVA

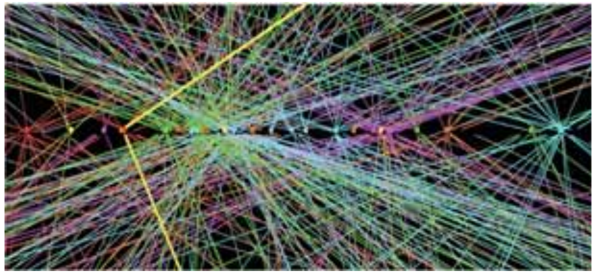


The ATLAS detector

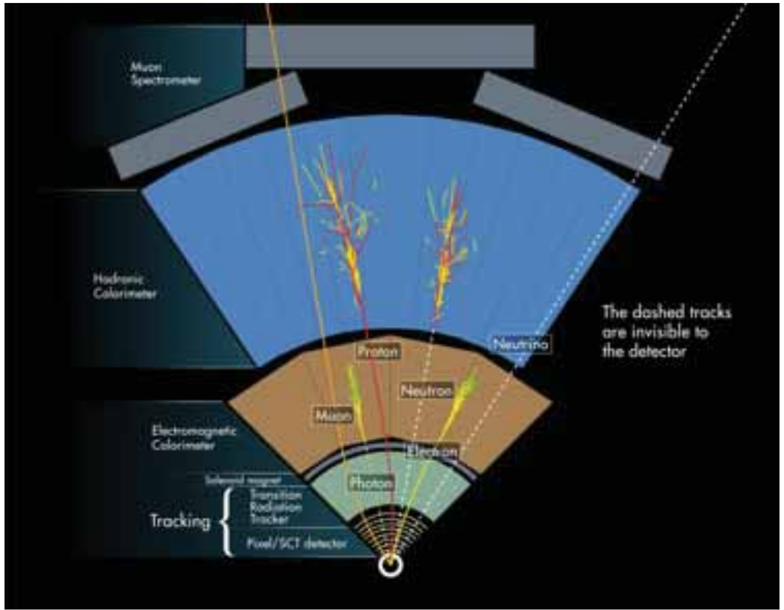


DATA COLLECTION

- **Hundreds of millions** of proton-proton collisions **per second**



- Filtered down to **400 events per second**
  - still **petabytes per year**
  - **real-time** (budgeted) classification: trigger
  - a research theme on its own

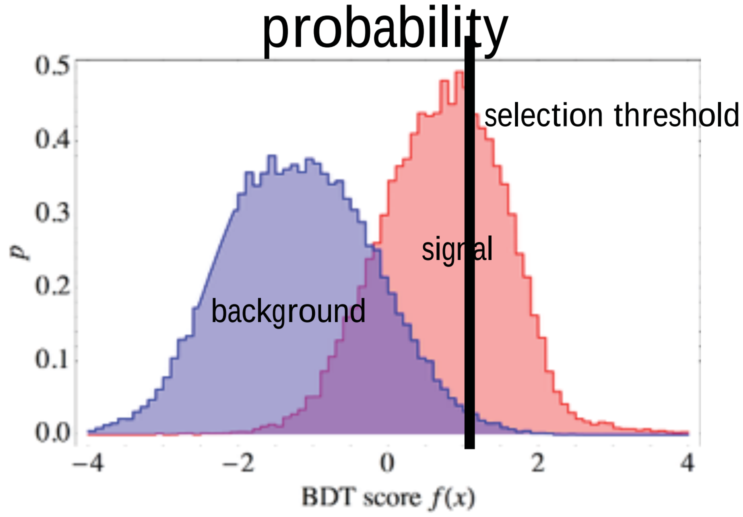


Feature engineering

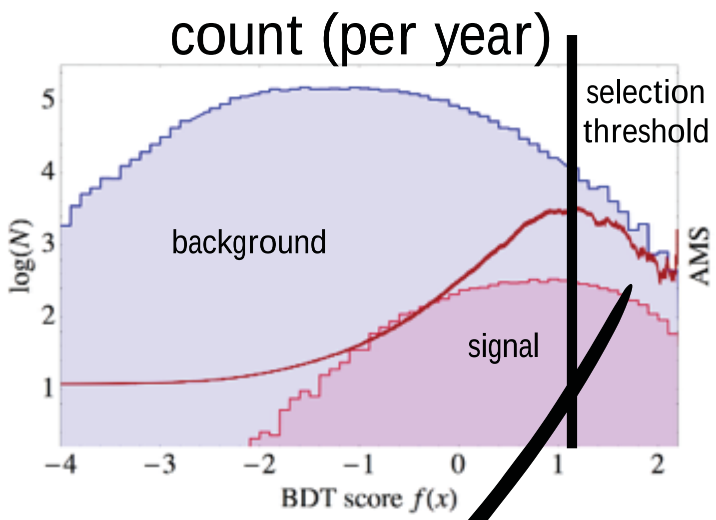
- Each collision is an **event**
  - **hundreds of particles**: decay products
  - **hundreds of thousands of sensors** (but sparse)
  - for each particle: **type**, **energy**, **direction** is measured
  - a fixed-length list of **~30-40 extracted features**: x
  - e.g., angles, energies, directions, reconstructed mass
  - based on **50 years** of accumulated **domain knowledge**

Classification for discovery

Goal: optimize the expected **discovery significance**



flux × time



total count,
say, 150 events

excess is $s = 50$ events

expected background
say $b = 100$ events

selection

$$\text{AMS} = \frac{s}{\sqrt{b}} = 5 \text{ sigma}$$

Generation and model reduction

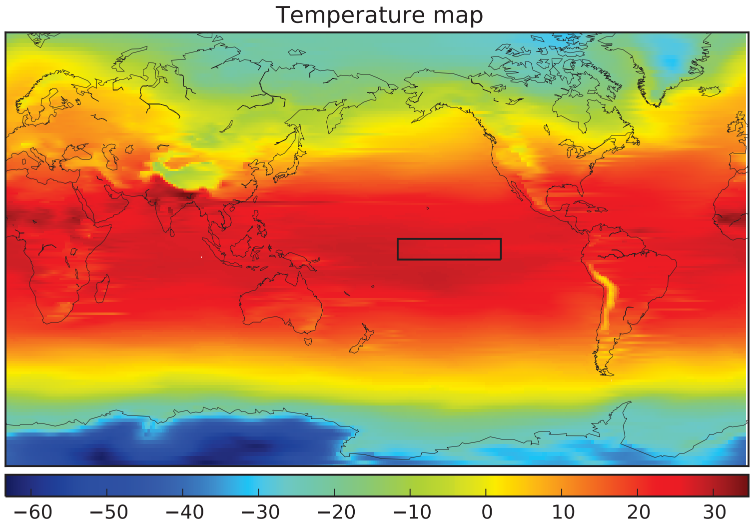
GENERATION AND MODEL REDUCTION

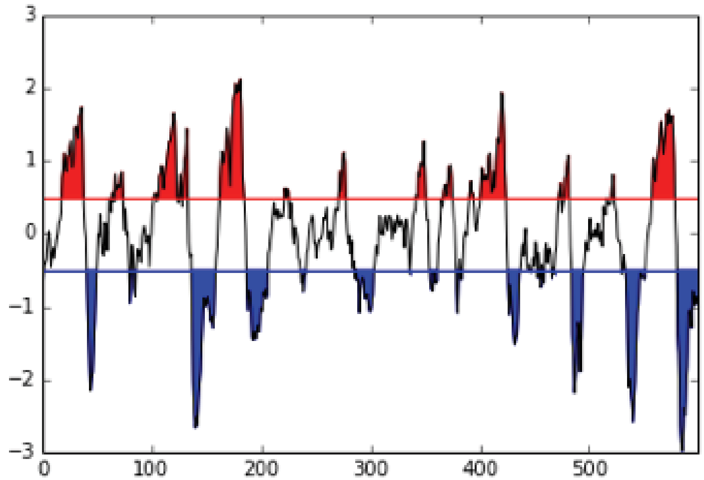
Why?

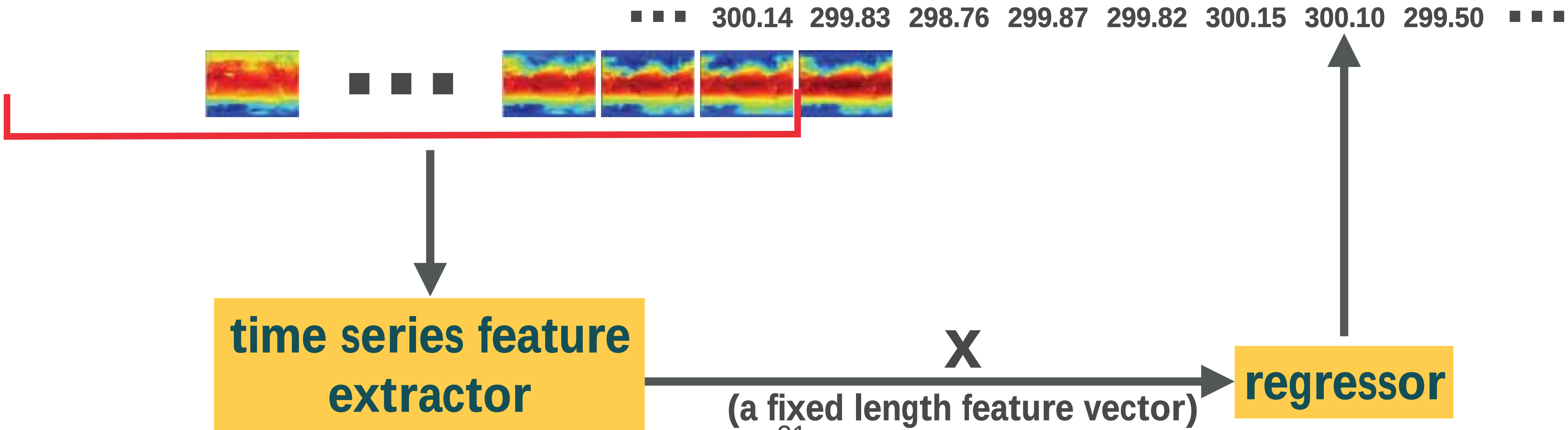
- Cost cutting 1: looking at the form of *f*, I can **place** my fixed number of **temperature sensors optimally**
- Cost cutting 2: *f* can replace costly simulation in a **detector optimization loop**
- Cost cutting 3: if I can generate realistic galaxy images, I can **replace costly manual labeling** of real photos

Forecasting El Nino: spatiotemporal time series

- collaboration with the **Climate Informatics workshop**
- also on **Arctic sea ice** and **California rainfall** prediction







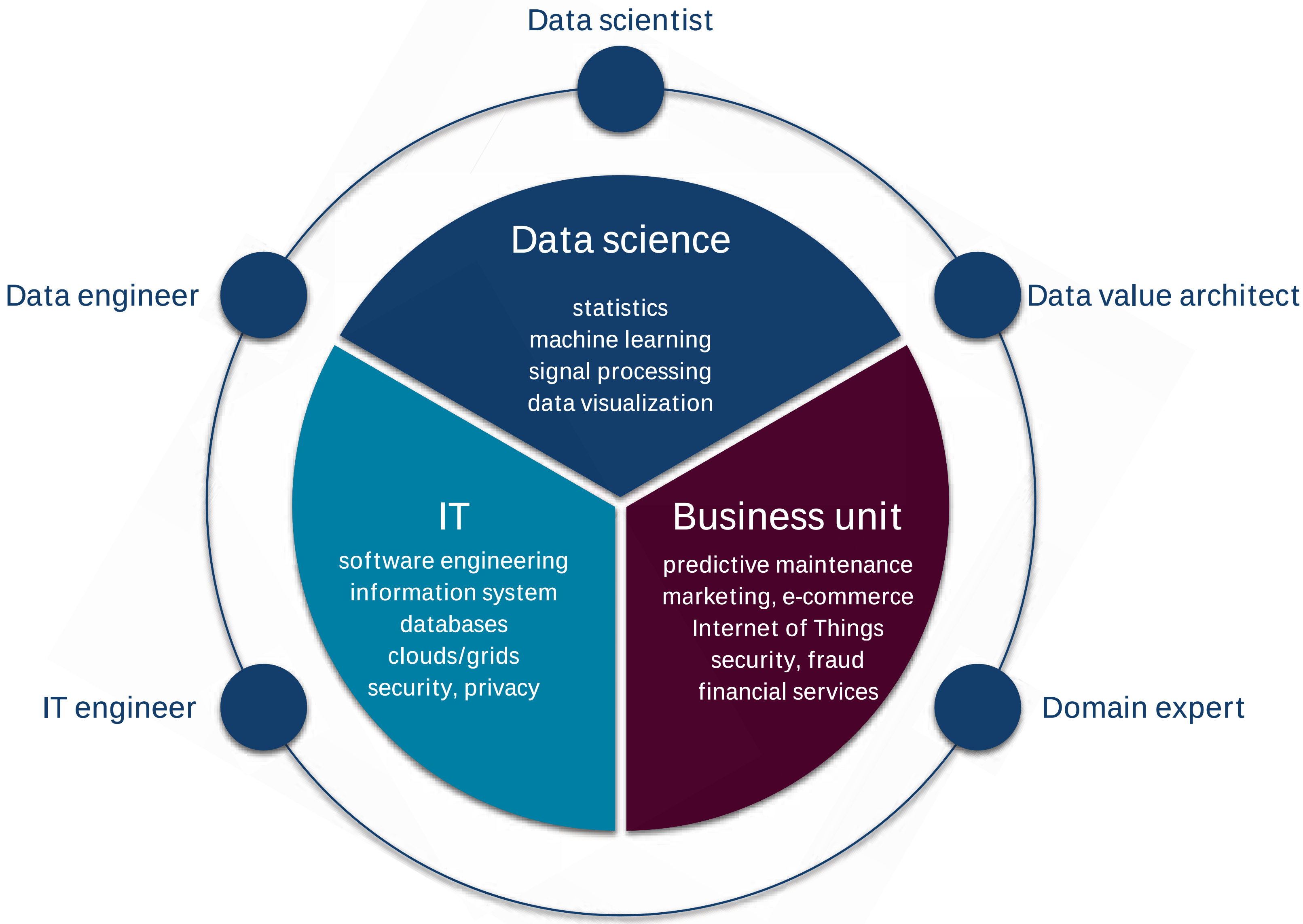
We have built and optimized
~20 scientific predictive workflows
for three years

What have we learned?

Building scientific workflows
what have we learned?

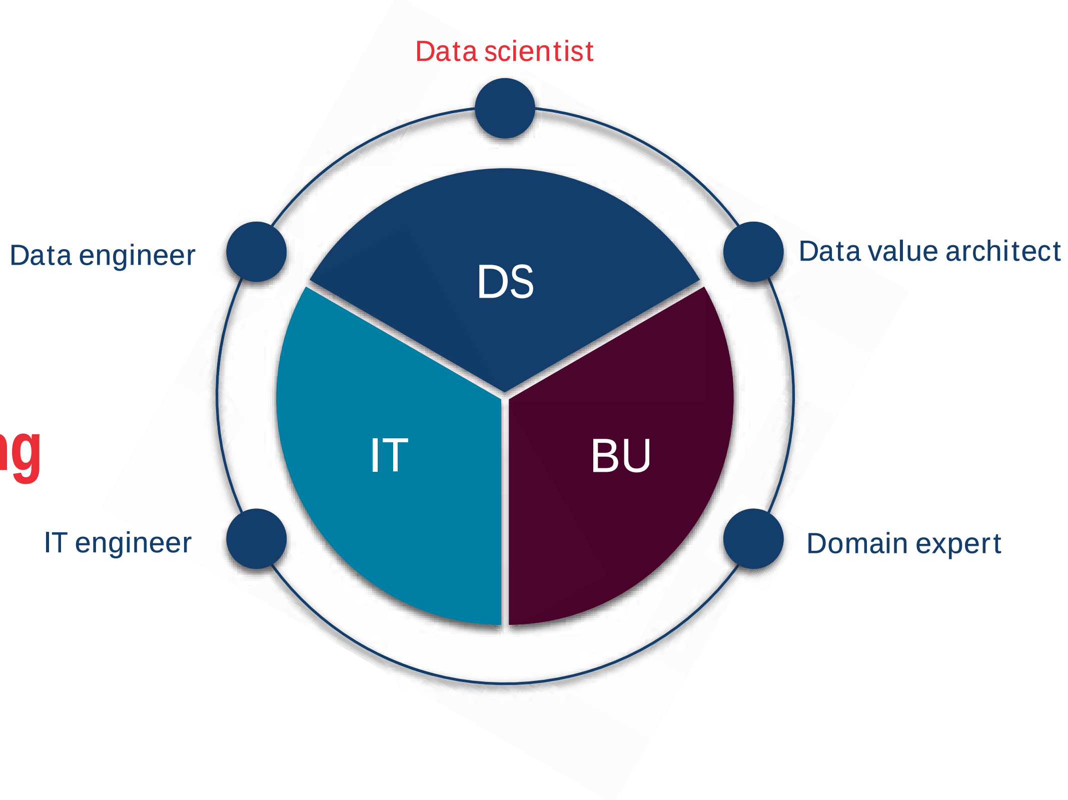
Roles and tasks in the data science process

The data science ecosystem

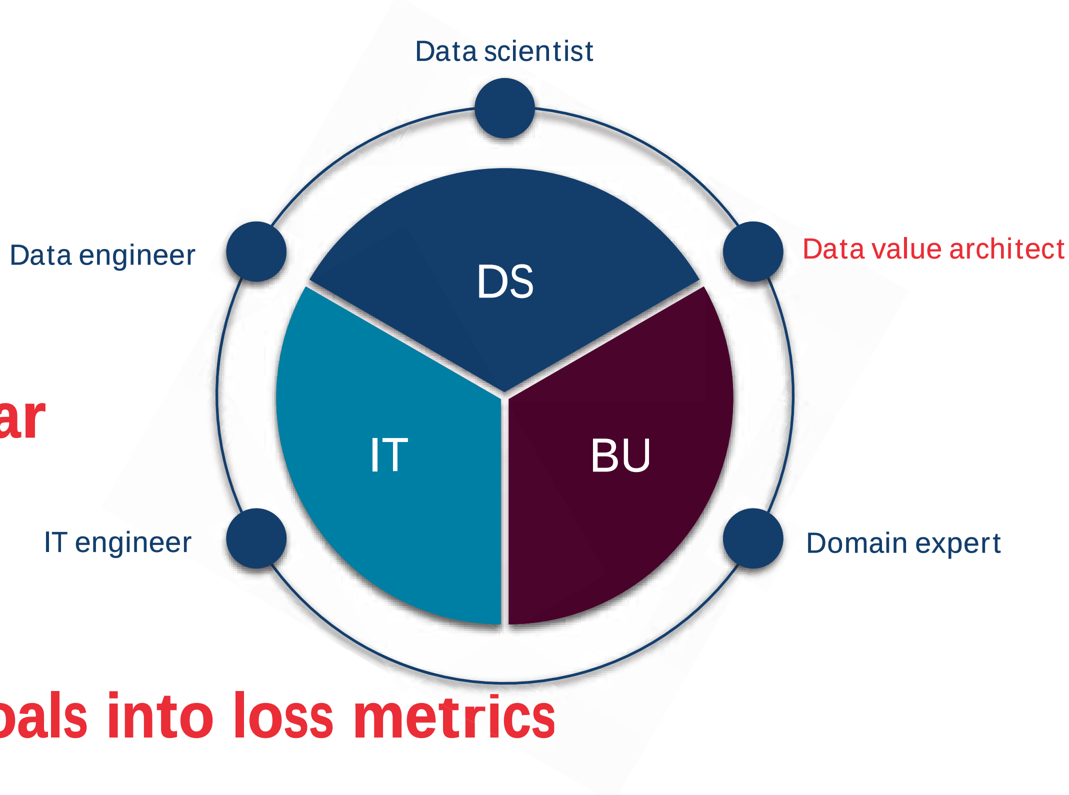


DATA SCIENTIST

- Technical expert in **machine learning**, **statistics**, **visualization**, **signal processing**
- Efficient in **cleaning** and **munging**
- Knows the latest **techniques** and **tools**
- Can handle different **data types** and **loss metrics**
- Can build adequate **prototype workflows**
- Knows how to **tune** (optimize) and **blend** models



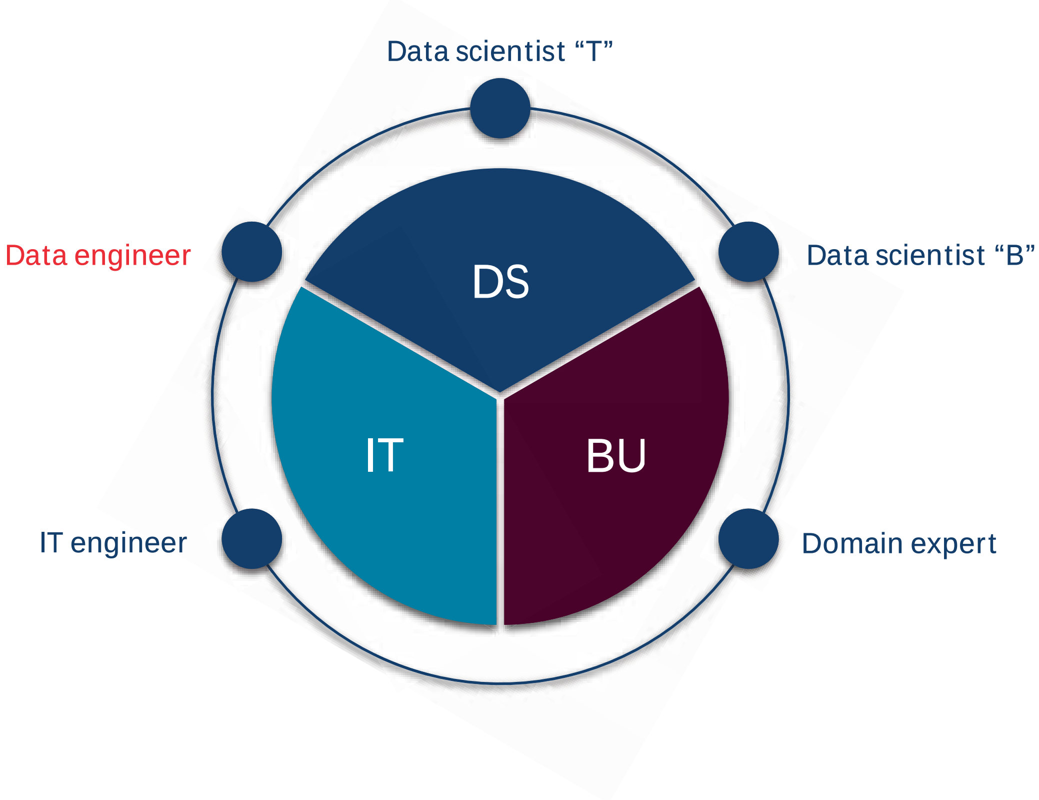
DATA VALUE ARCHITECT



- Has experience with a **wide variety of problems** and **technical solutions**
- Is possibly **expert in the particular domain**, or at least can **converse** with the domain expert
- Can translate **business/science goals into loss metrics**
- Can **formalize** adequate **prototype workflows**
- Can **estimate the costs** of building and running workflows
- Can define and dimension the **data collection** effort

DATA ENGINEER

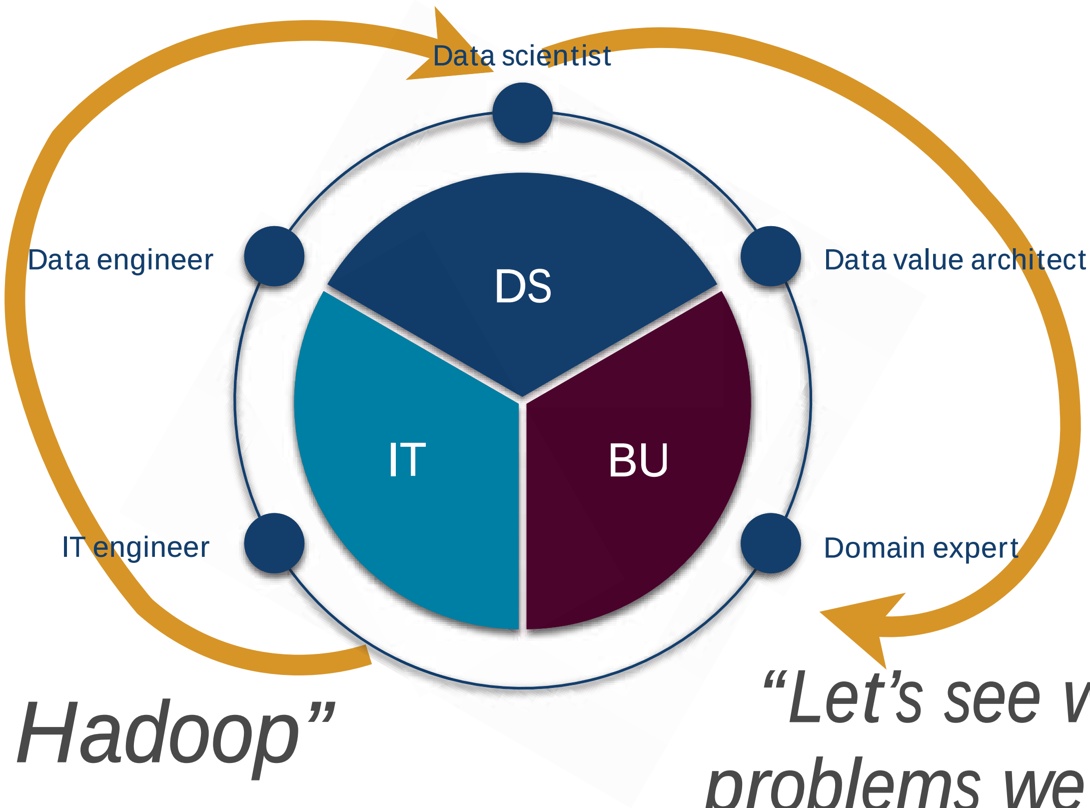
- Translates prototypes into **production workflows**, runs and maintains them
- Knows the latest **data engineering systems** and **architectures**
- Knows the **existing IT**
- Can **dimension the production workflows** and **estimate their costs**
- Knows the **basics of building** a data science workflow, and can feed the process by **extracting** and possibly **cleaning/munging** adequate data



université PARIS-SACLAY
Paris-Saclay Center for Data Science

BUILDING A DATA SCIENCE ECOSYSTEM DRIVEN BY IT

"Let's hire data scientists"

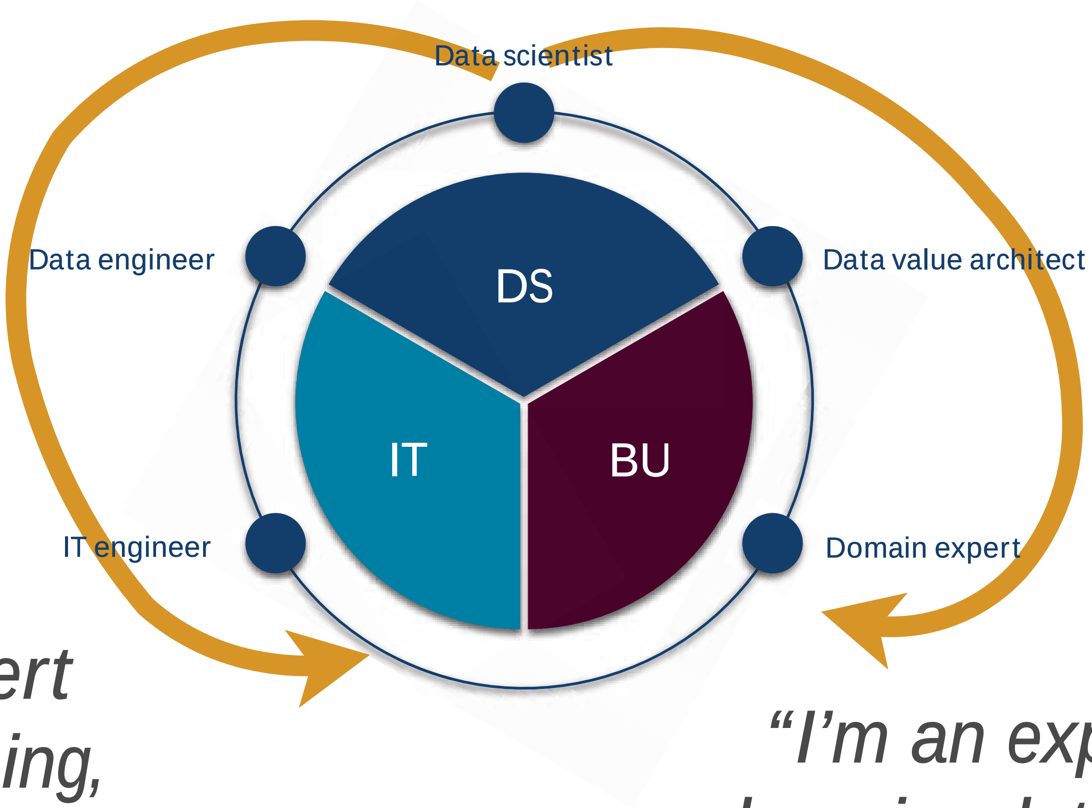


"Let's install Hadoop"

"Let's see what business problems we can solve with the existing data science team and the infrastructure we bought"

BUILDING A DATA SCIENCE ECOSYSTEM DRIVEN BY DATA SCIENTISTS

"Let's hire data scientists."

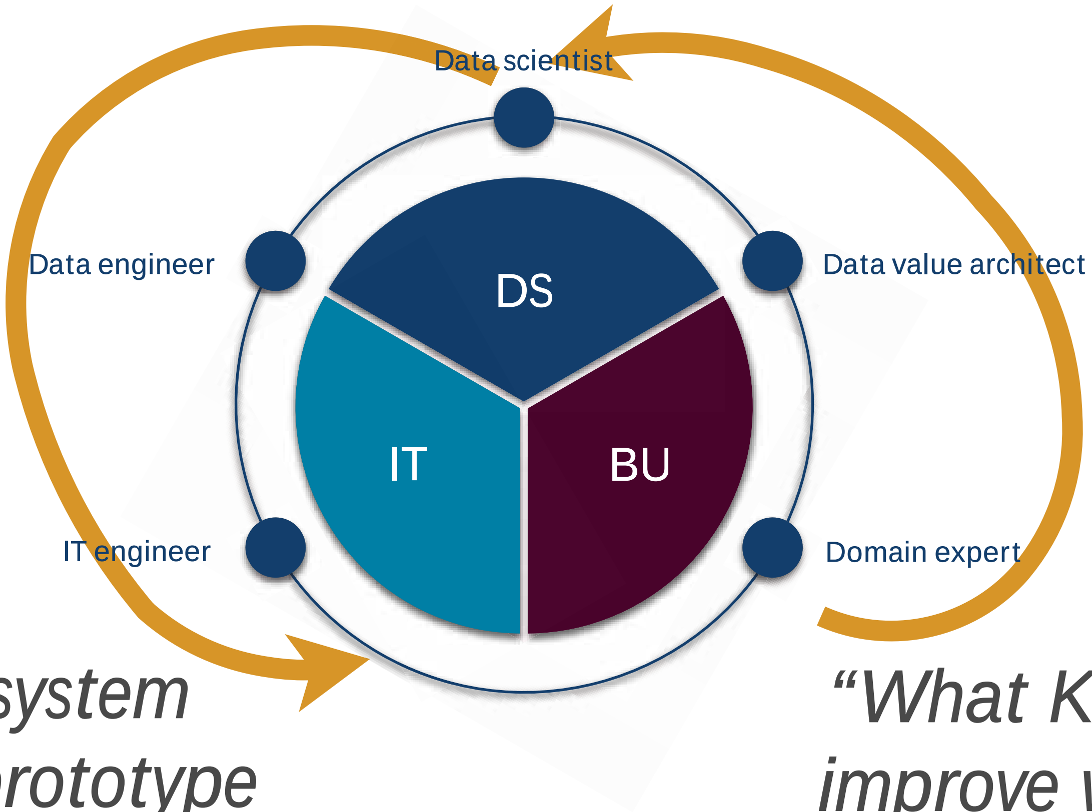


"I'm an expert of deep learning, let's by a GPU cluster."

"I'm an expert of deep learning, let's see what it can do for your business."

Building a data science ecosystem driven by business

"Let's hire data scientists for prototyping the business case."

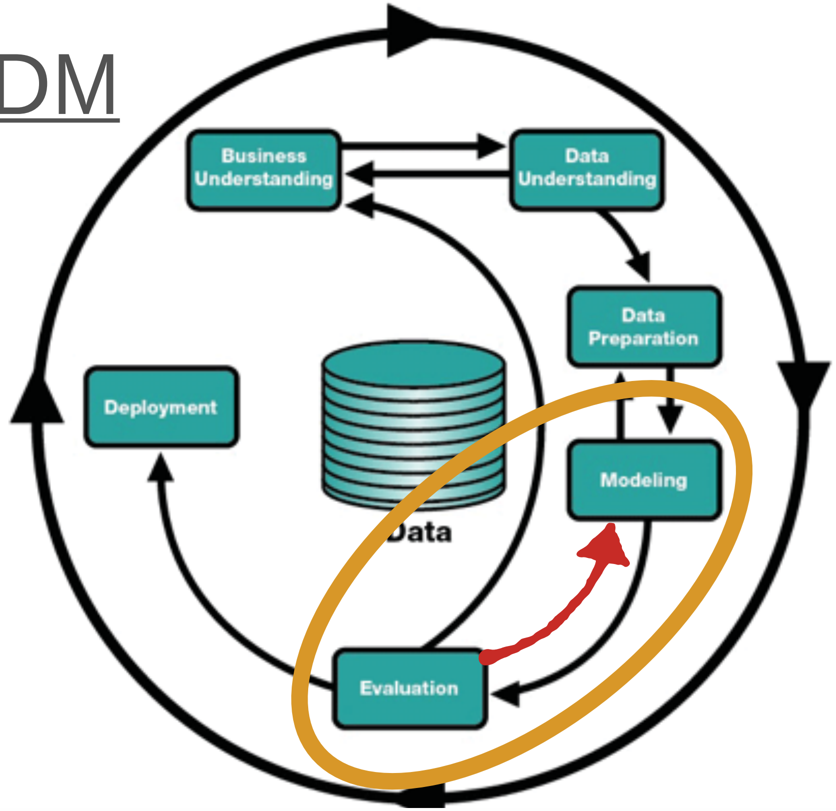


"Let's build a system for putting the prototype into production."

"What KPI can we improve with data? What data should we collect?"

BUILDING PREDICTIVE SOLUTIONS

IBM CRISP-DM



1996

2016

Dataiku

THE DATA ANALYTICS BUILDING PIPELINE

WHO DOES WHAT AND WHEN

business expert + data value architect

80% **20%**

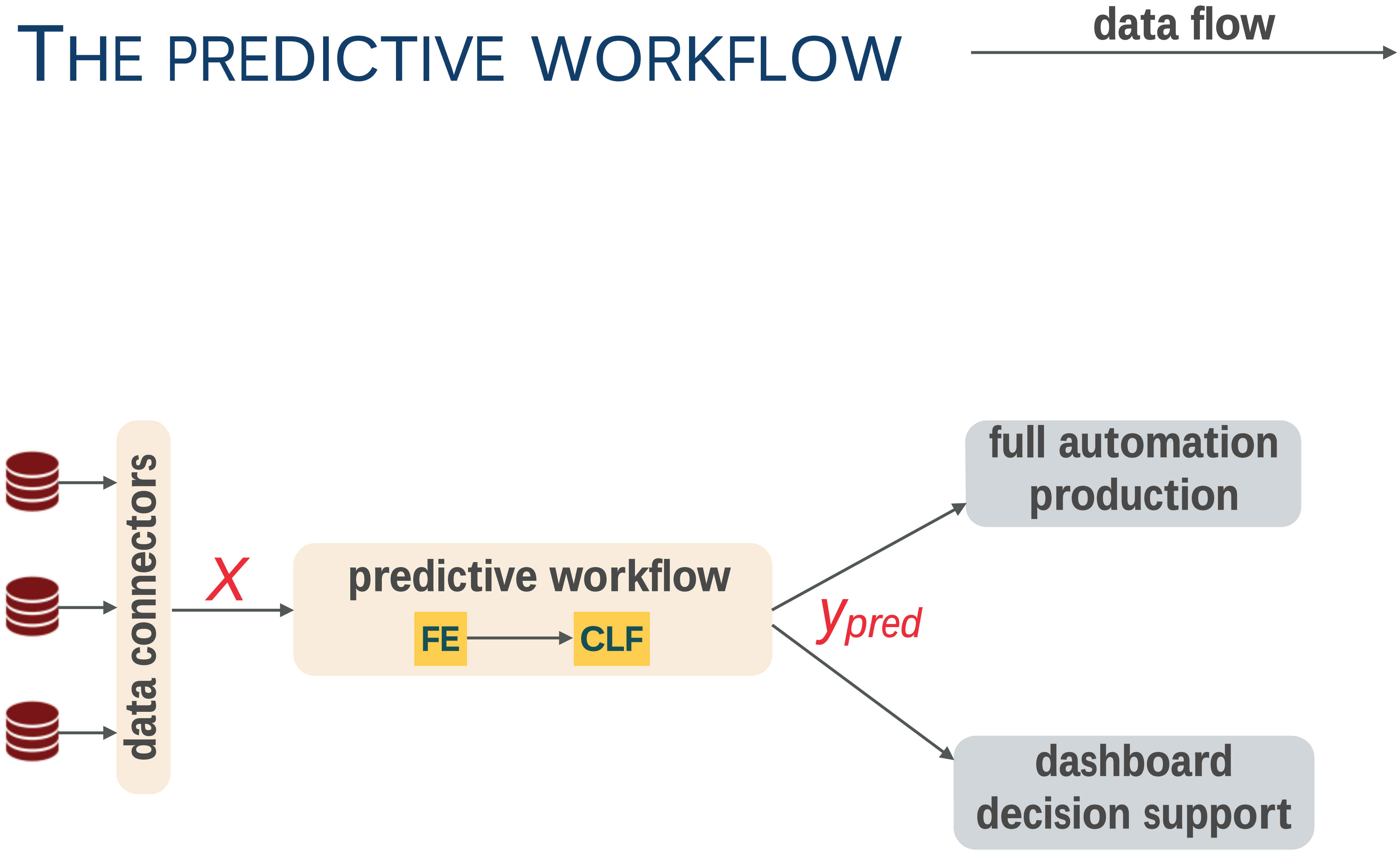
data scientist

data engineer (+ business expert)

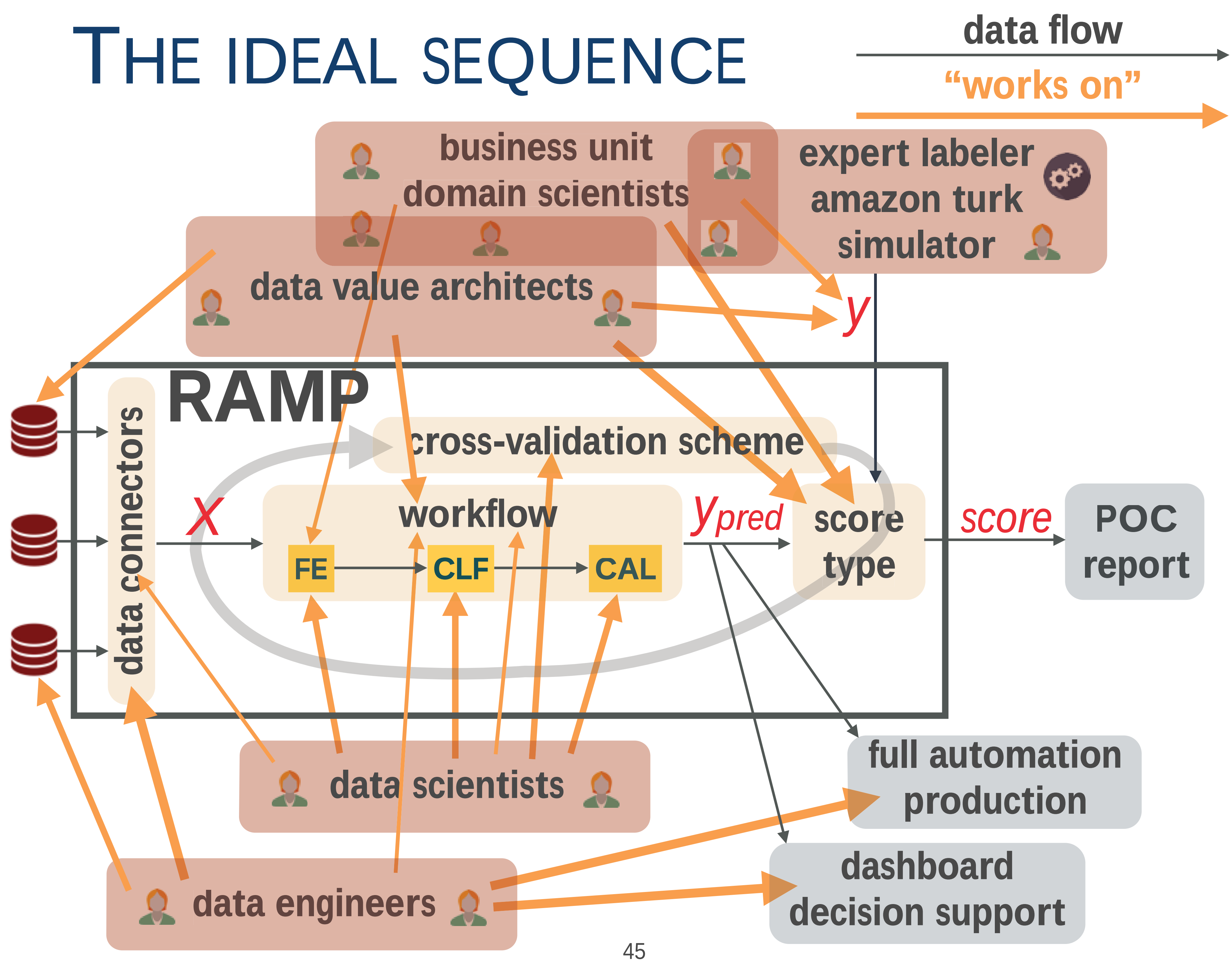
Building scientific workflows what have we learned?

Building the workflow:
what are the tasks and who does what

THE PREDICTIVE WORKFLOW



THE IDEAL SEQUENCE



BUILDING THE PREDICTIVE WORKFLOW

- It is **trial and error**
  - little if any theory-based, model-based design
  - even research (development of new algorithms) is (mostly) trial and error
  - the data scientist's best friend is a **well-designed experimental studio** for facilitating fast iterations of
    - what **data** to use
    - what **features** to select or engineer
    - what **predictors** to use
    - how to **parametrize** the predictors

Building scientific workflows
what have we learned?

What is a predictive workflow?

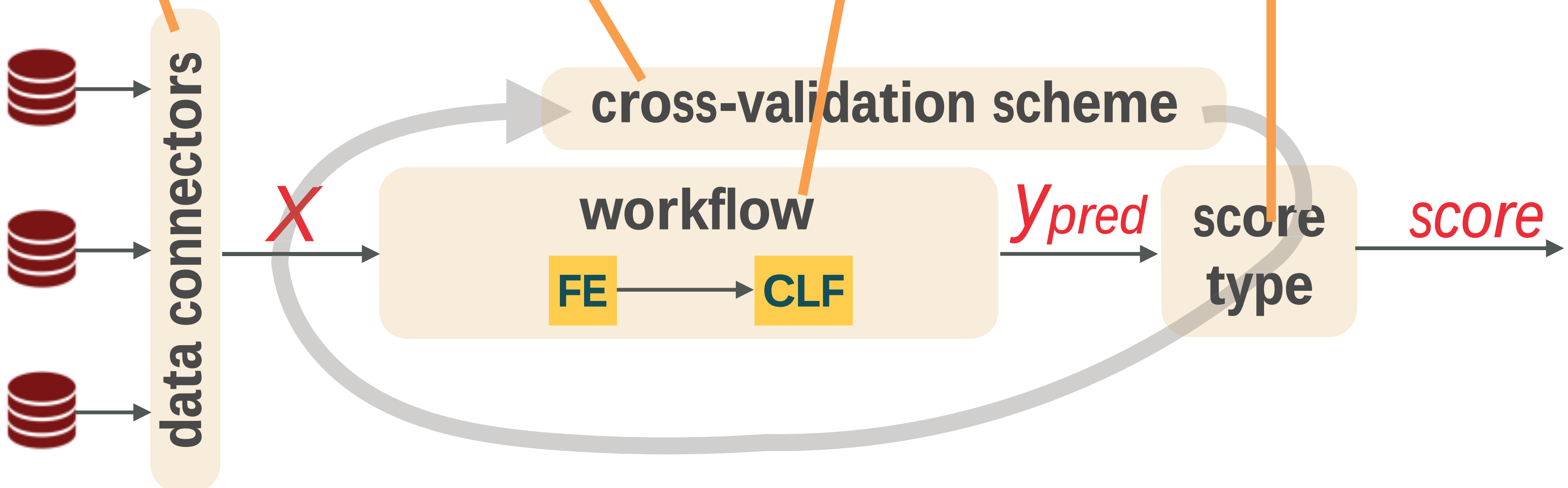
What are the parametrizable components?

What can be put into a
unique training/scoring script?

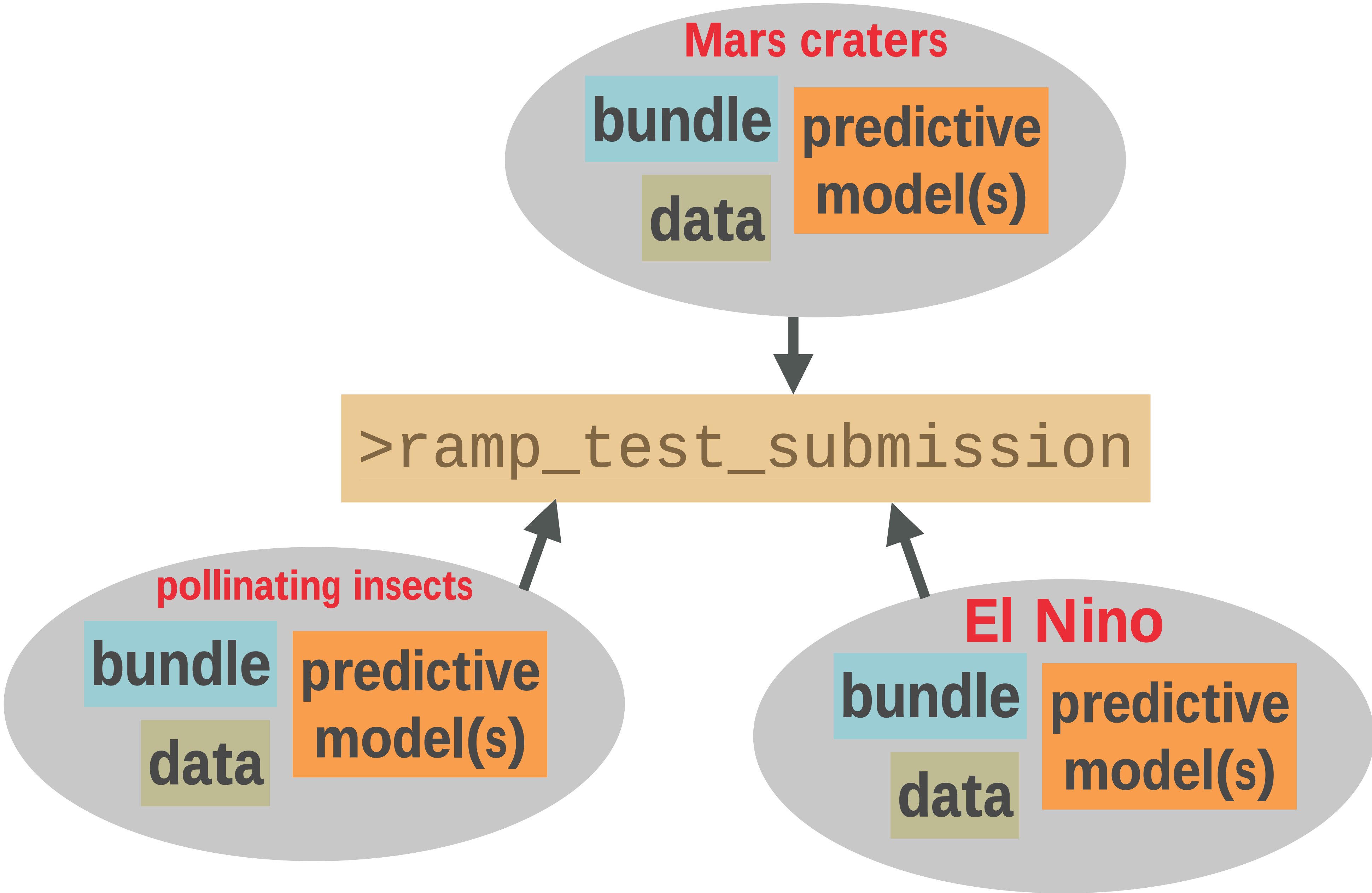
A SINGLE SCRIPT TO DEFINE THE BUNDLE

```python


def get_cv(X, y):
    unique_replicates = np.unique(X['replicate'])
    r = np.arange(len(X))
    for replicate in unique_replicates:
        train_is = r[(X['replicate'] != replicate).values]
        test_is = r[(X['replicate'] == replicate).values]
        yield train_is, test_is


def _read_data(path, f_name):
    data = pd.read_csv(os.path.join(path, 'data', f_name))
    y_array = data[_target_column_name]
    X_df = data.drop([_target_column_name], axis=1)
    return X_df, y_array


def get_train_data(path='.'):
    f_name = 'train.csv.gz'
    return _read_data(path, f_name)


def get_test_data(path='.'):
    f_name = 'test.csv.gz'
    return _read_data(path, f_name)
```

```python
import os
import numpy as np
import pandas as pd
import rampwf as rw

problem_title =
    'Cell population identification from single-cell mass cytometry data'
_target_column_name = 'cell type'
_prediction_label_names = [
    'B-cell Frac A-C (pro-B cells)', 'Basophils', 'CD4 T cells', 'CD8 T cells',
    'CLP', 'CMP', 'Classical Monocytes', 'Eosinophils', 'GMP', 'HSC',
    'IgD- IgMpos B cells', 'IgDpos IgMpos B cells', 'IgM- IgD- B-cells',
    'Intermediate Monocytes', 'MEP', 'MPP', 'Macrophages', 'NK cells',
    'NKT cells', 'Non-Classical Monocytes', 'Plasma Cells', 'gd T cells',
    'mDCs', 'pDCs']
# A type (class) which will be used to create wrapper objects for y_pred
Predictions = rw.prediction_types.make_multiclass(
    label_names=_prediction_label_names)
# An object implementing the workflow
workflow = rw.workflows.FeatureExtractorClassifier()

score_types = [
    rw.score_types.BalancedAccuracy(name='bac', precision=3),
    rw.score_types.Accuracy(name='acc', precision=3),
    rw.score_types.NegativeLogLikelihood(name='nll', precision=3),
]
```



A unique script to run the bundles



A UNIQUE SCRIPT TO RUN THE BUNDLES

```
1 read training and test data
2 read submission
3 create train and valid folds
  on training data
4 for all train and valid folds:
5     train submission on train
6     score submission on train,
      valid, and test
7 summarize scores
```

```
silver6:autism kegl$ ramp_test_submission
Testing Autism Spectrum Disorder classification
Reading train and test files from ./data ...
Reading cv ...
Training ./submissions/starting_kit ...
CV fold 0
Couldn't re-order the score matrix..
        score   acc    auc
        test    0.696  0.765
        train   0.767  0.847
        valid   0.611  0.647
CV fold 1
Couldn't re-order the score matrix..
        score   acc    auc
        test    0.478  0.659
        train   0.766  0.842
        valid   0.628  0.662
CV fold 2
Couldn't re-order the score matrix..
        score   acc    auc
        test    0.609  0.720
        train   0.786  0.854
        valid   0.615  0.645
CV fold 3
Couldn't re-order the score matrix..
        score   acc    auc
        test    0.565  0.758
        train   0.769  0.849
        valid   0.619  0.645
----------------------------
Mean CV scores
----------------------------
Couldn't re-order the score matrix..
        score            acc               auc
        test    0.587 ± 0.0784    0.725 ± 0.042
        train   0.772 ± 0.0081   0.848 ± 0.0042
        valid   0.618 ± 0.0065    0.65 ± 0.0072
----------------------------
Bagged scores
----------------------------
Couldn't re-order the score matrix..
        score   auc
        test    0.735
        valid   0.647
```

RAMP-WORKFLOW & RAMP-KITS

- toolkit: https://github.com/paris-saclay-cds/**ramp-workflow**
  - for **designing workflows**
  - set of ready-made **metrics, workflows, CV schemes,** data readers
  - unique command-line **test script**
- examples: https://github.com/**ramp-kits**
  - a zoo of **problems**, **experiments**, **workflows**
  - (at least) one **initial solution**

Building scientific workflows
what have we learned?

How to make
(novice) data scientists efficient

How to make data scientists efficient

- Principles
  - **incite them** to work on the problem
  - give them a working (but unoptimized) **model to start with**
  - make **incremental contributions** easy
  - **gamify optimization**
  - help them to **collaborate** and to **learn from each other**
  - **“hide” heavy engineering** and computational obstacles

The Jupyter notebook

Paris Saclay Center for Data Science

RAMP on Pollinating insect classification

Mehdi Cherti (CNRS), Romain Julliard (MNHN), Gregoire Lois (MNHN), Balázs Kégl (CNRS)

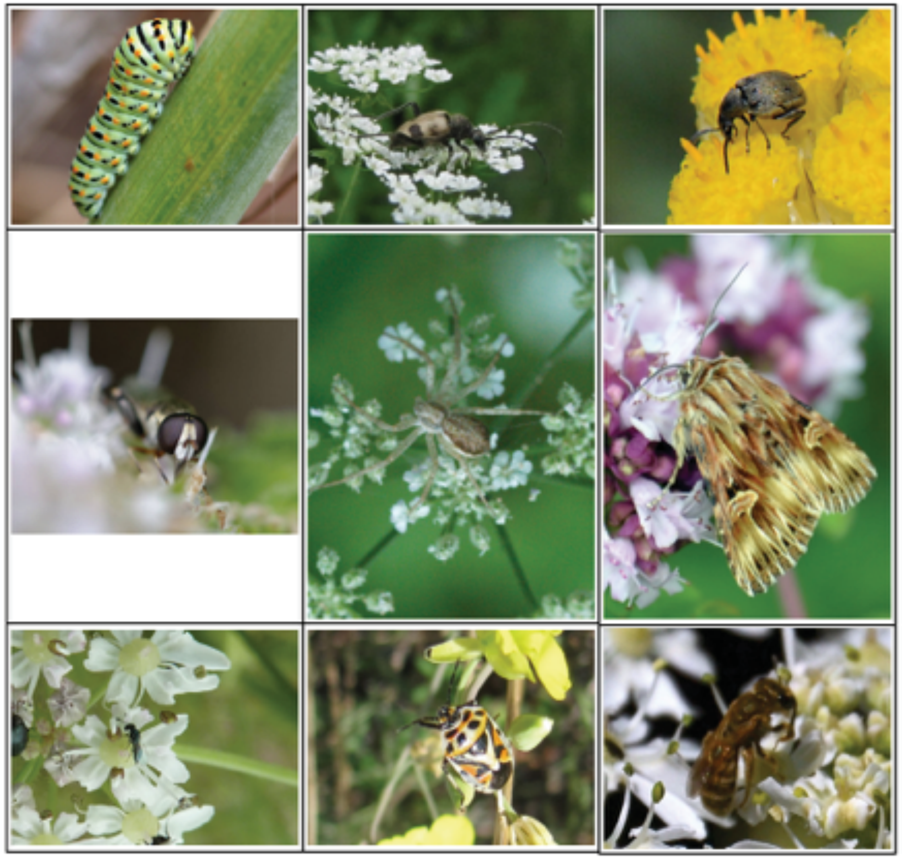
Introduction

Pollinating insects play a fundamental role in the stability of ecosystems. An insect is said to be pollinator when it transports pollen from one flower to another, helping them to accomplish fertilization. The vast majority of plants pollinates using insects, and at the same time, these insects depend on plants for their survival. However, because of human intensified agriguture, urbanisation and climate change, these species are threatened. 35% of human alimentation is based on plants pollinated by insects. Diversity of these insects is also important, the more diverse they are the best overall assistance is provided by these insects.

The SPIPOLL (Suivi Photographique des Insectes POLLinisateurs) project proposes to quantitatively study pollinating insects in France. For this, they created a crowdsourcing platform where anyone can upload pictures of insects and identify their species through a series of questions. These data are then used by specialists for further analyses.

Data

In this RAMP, we propose a dataset of pictures of insects from different species gathered from the SPIPOLL project and labeled by specialists. The dataset contains a set of 72939 labeled pictures of insects coming from 403 different insect species. Each picture is a color image. The size of the images (number of pixels) vary.



The prediction task

[
](http://www.datascience-paris-saclay.fr)

RAMP on Mars craters detection

Alexandre Boucaud (CDS), Joris van den Bossche (CDS), Balazs Kegl (CDS), Frédéric Schmidt (GEOPS), Anthony Lagain (GEOPS)

1. Introduction
2. Preprocessing
3. Workflow
4. Evaluation
5. Local testing/exploration
6. Submission

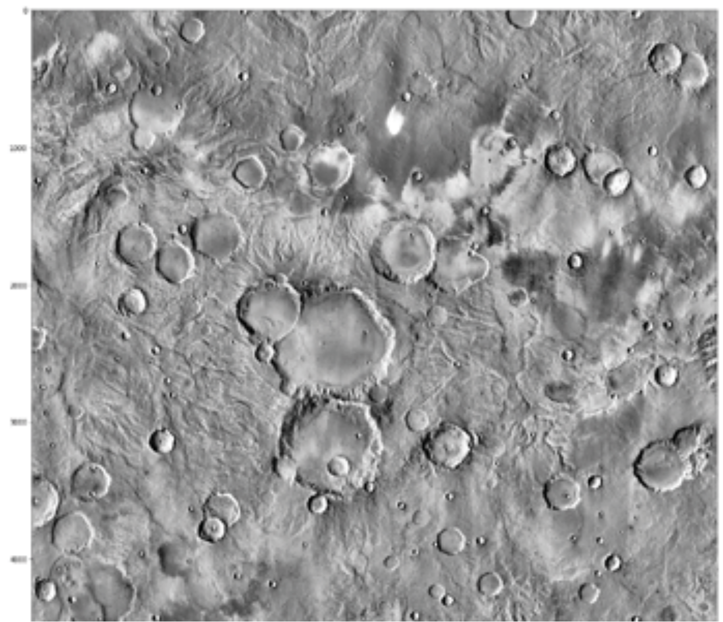
Introduction

Impact craters in planetary science are used to date planetary surfaces, to characterize surface processes and to study the upper crust of terrestrial bodies in our Solar System (Melosh, 1989). Thanks to the Martian crater morphology, a wide amount of information could be deduced on the geological history of Mars, as for example the evolution of the surface erosion rate, the presence of liquid water in the past, the volcanic episodes or the volatiles layer in the subsurface (Carr & Head, 2010). These studies are widely facilitated by the availability of reference crater databases.

Surveying impact craters is therefore an important task which traditionally has been achieved by means of visual inspection of images. The enormous number of craters smaller than one kilometer in diameter, present on high resolution images, makes visual counting of such craters impractical. In order to overcome this problem, several algorithms have been developed to automatically detect impact structures on planetary images (Bandeira et al., 2007 ; Martins et al., 2009). Nevertheless, these method allow to detect only 70-80 % of craters (Urbach & Stepinski, 2009).

The prediction task

This challenge proposes to design the best algorithm to detect crater position and size starting from the most complete Martian crater database containing 384 584 verified impact structures larger than one kilometer of diameter (Lagain et al. 2017). We propose to give to the users a subset of this large dataset in order to test and calibrate their algorithm.



THE STARTING KIT

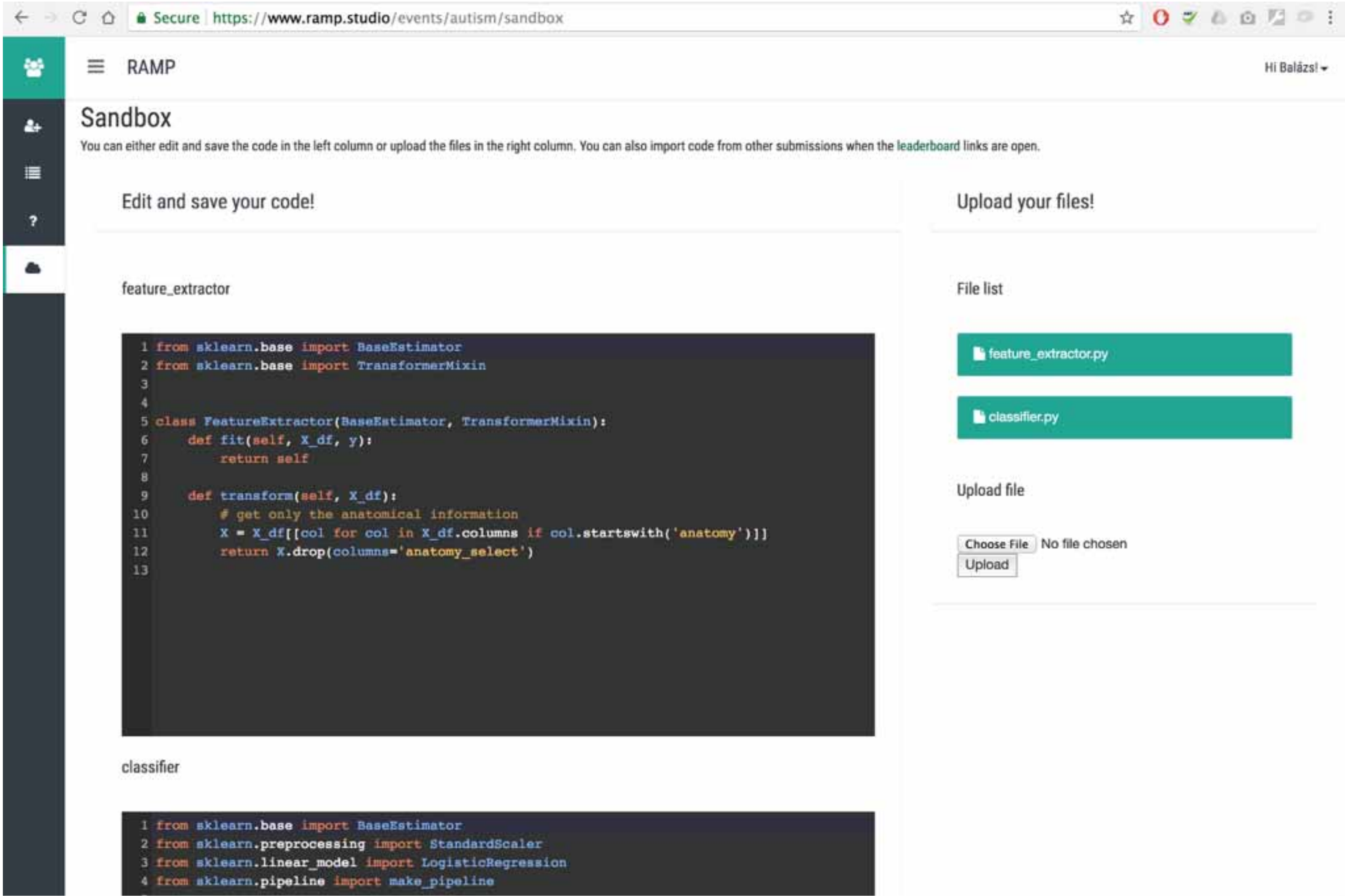
feature_extractor.py

```python
from sklearn.base import BaseEstimator
from sklearn.base import TransformerMixin


class FeatureExtractor(BaseEstimator, TransformerMixin):
    def fit(self, X_df, y):
        return self

    def transform(self, X_df):
        # get only the anatomical information
        X = X_df[[
            col for col in X_df.columns
            if col.startswith('anatomy')]]
        return X.drop(columns='anatomy_select')
```

classifier.py

```python
from sklearn.base import BaseEstimator
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import make_pipeline


class Classifier(BaseEstimator):
    def __init__(self):
        self.clf = make_pipeline(
            StandardScaler(), LogisticRegression(C=1.))

    def fit(self, X, y):
        self.clf.fit(X, y)
        return self

    def predict(self, X, y):
        return self.clf.predict(X)

    def predict_proba(self, X):
        return self.clf.predict_proba(X)
```

THE FRONTEND



THE LEADERBOARD

Secure | https://www.ramp.studio/events/autism/competition_leaderboard

RAMP

Hi Balázs!

autism

Leaderboard

Combined score: 1.0

Show 10 entries

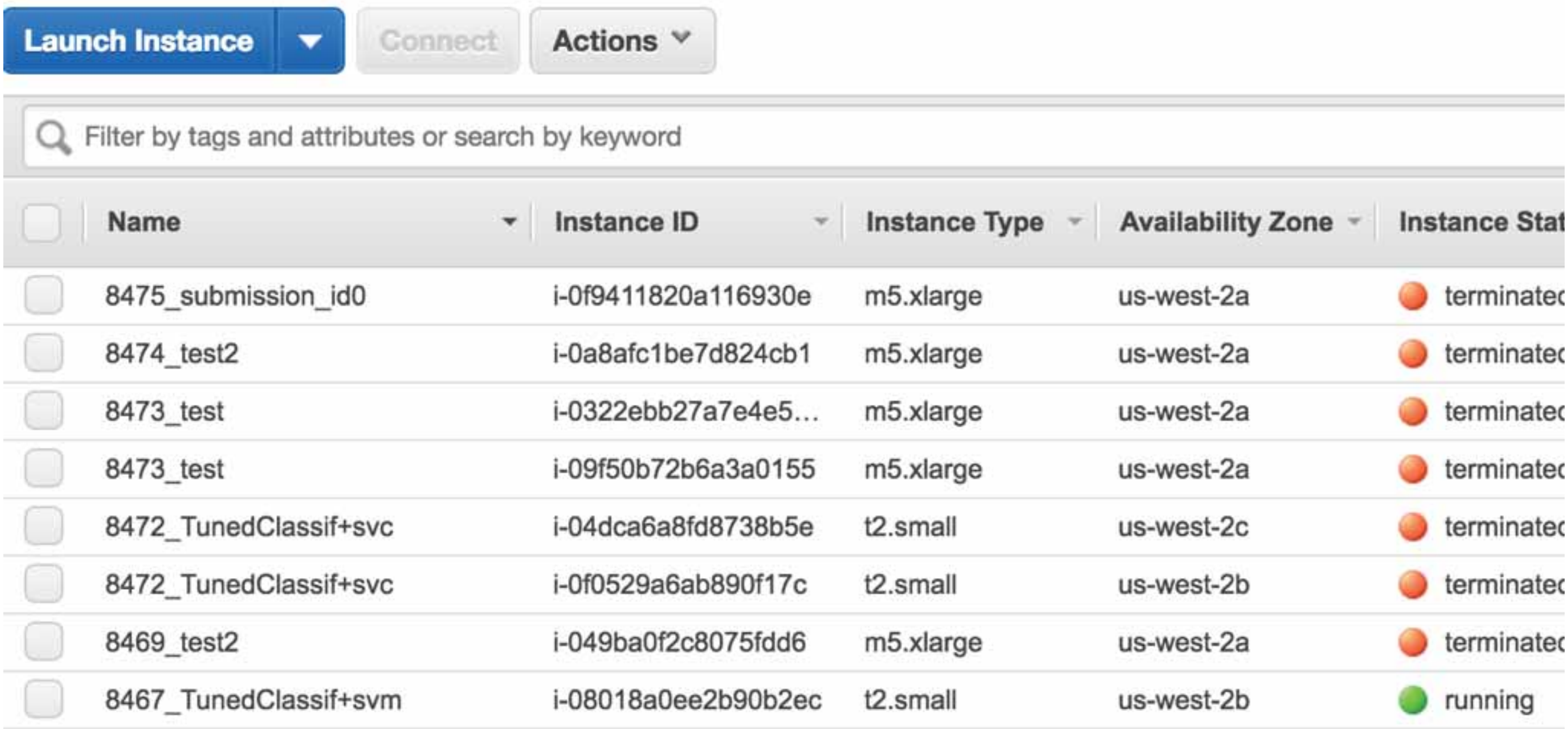
Search:

rank	team	submission	auc	train time [s]	test time [s]	submitted at (UTC)
1	Warvito	sub_EP	0.997	151	29	2018-06-18 21:21:25 Mon
2	vfdev.5	lr_f23_fmri_nv=0.998	0.996	50	50	2018-06-16 17:18:28 Sat
3	jmr	test13	0.976	559	149	2018-06-15 10:40:37 Fri
4	pearrr	test9	0.948	786	153	2018-06-18 13:40:47 Mon
5	Gowtham_Murugesan	test_009	0.934	695	202	2018-06-13 17:05:50 Wed
6	nherran	test_22_part_4	0.908	350	131	2018-06-12 18:16:51 Tue
7	zhipeng	con_test1_1	0.806	542	170	2018-06-22 12:37:56 Fri
8	mmunoz	subm_3	0.776	152	71	2018-06-22 22:25:54 Fri
9	wwwwmmmm	mengxb-3	0.772	773	50	2018-06-06 01:01:45 Wed
10	SRSteinkamp	2atl_mlp	0.772	72	26	2018-06-18 04:50:24 Mon

Showing 1 to 10 of 39 entries

Previous 1 2 3 4 Next

The backend on Amazon Web Services



Name	Instance ID	Instance Type	Availability Zone	Instance Stat
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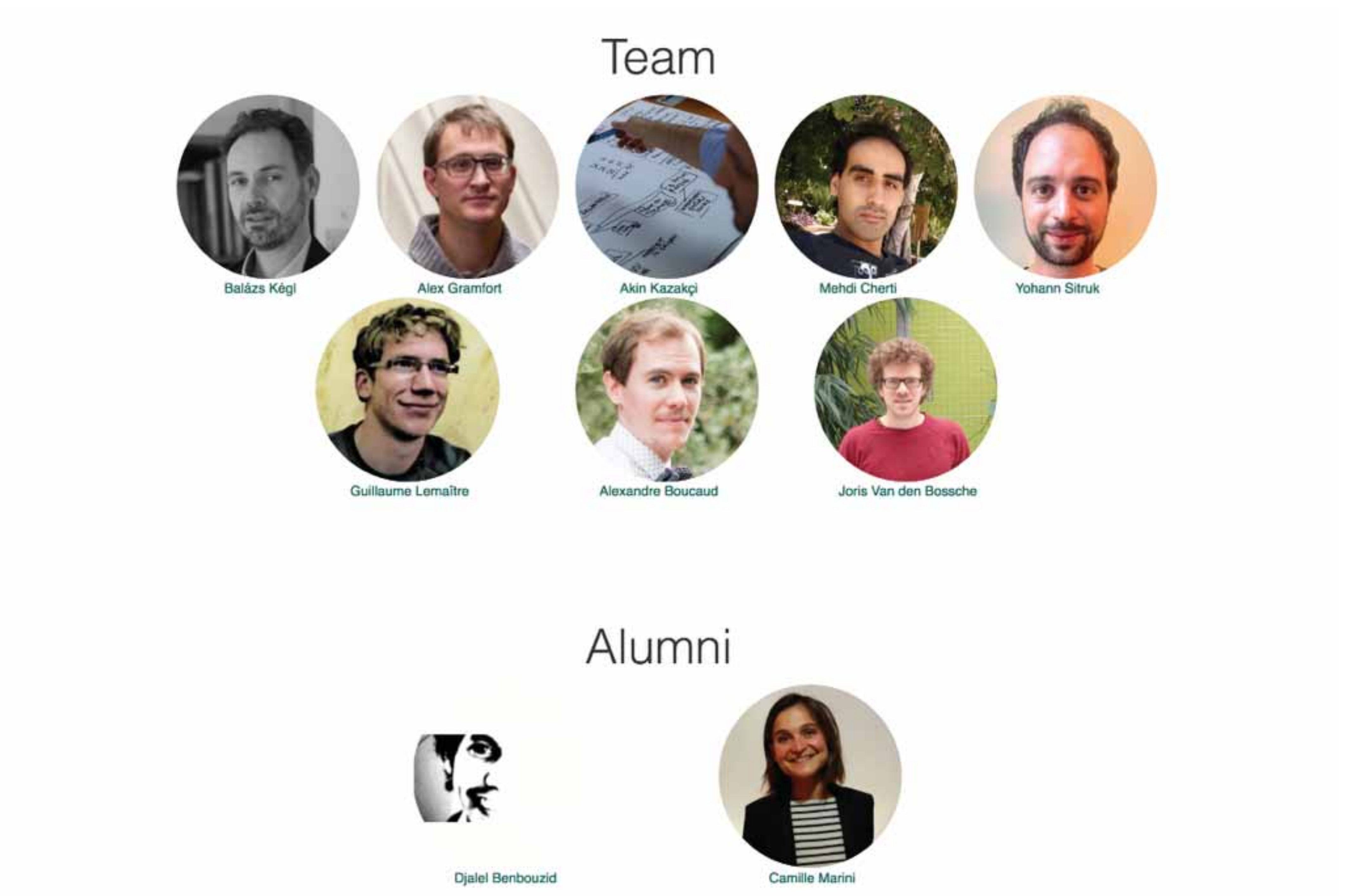
8474_test2	i-0a8afc1be7d824cb1	m5.xlarge	us-west-2a	terminatec
8473_test	i-0322ebb27a7e4e5...	m5.xlarge	us-west-2a	terminatec
8473_test	i-09f50b72b6a3a0155	m5.xlarge	us-west-2a	terminatec
8472_TunedClassif+svc	i-04dca6a8fd8738b5e	t2.small	us-west-2c	terminatec
8472_TunedClassif+svc	i-0f0529a6ab890f17c	t2.small	us-west-2b	terminatec
8469_test2	i-049ba0f2c8075fdd6	m5.xlarge	us-west-2a	terminatec
8467_TunedClassif+svm	i-08018a0ee2b90b2ec	t2.small	us-west-2b	running

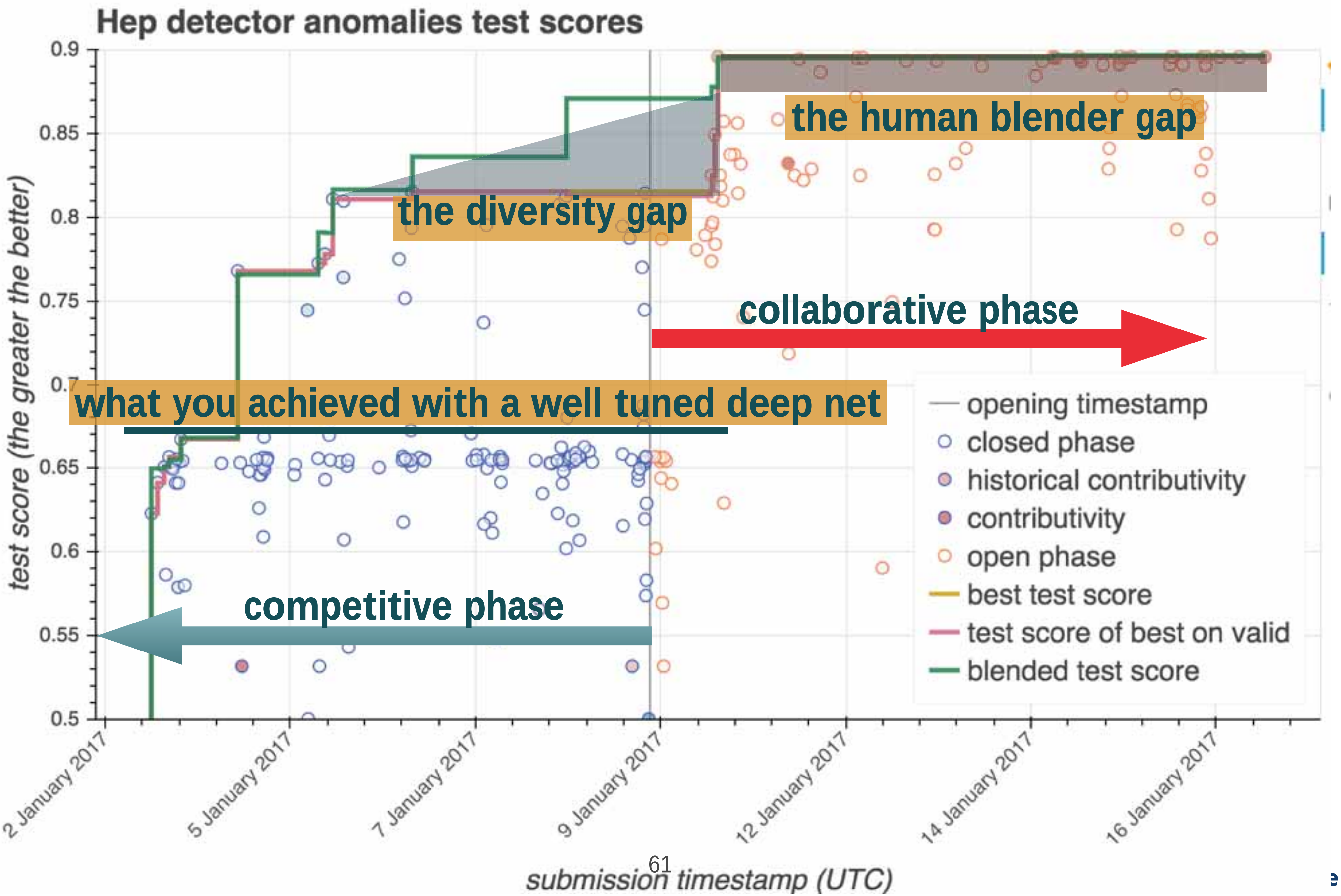
Funded by Université Paris-Saclay and CNRS



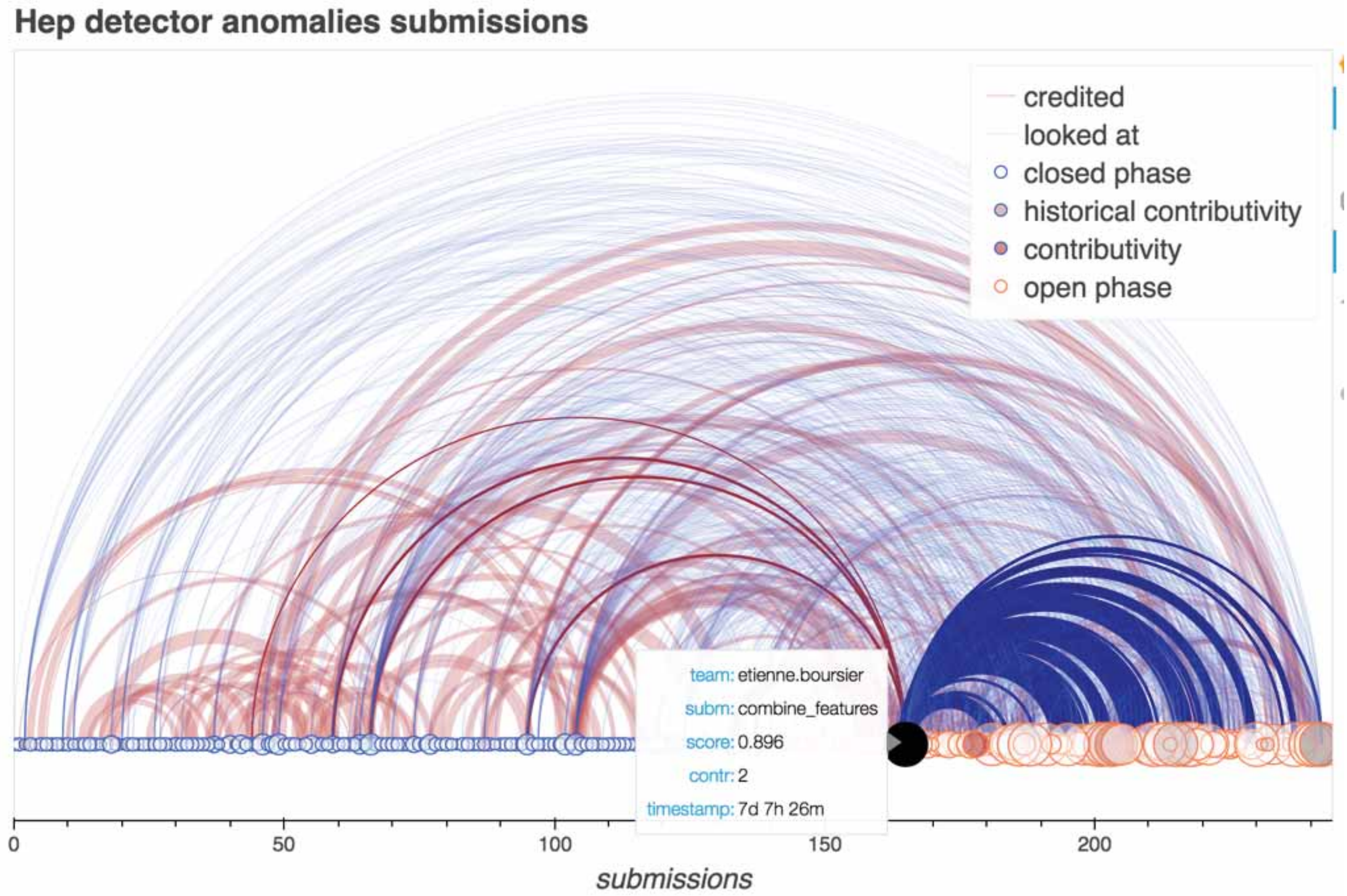
Why code submission

1. lets us deliver a **working prototype**
2. lets the participants **collaborate**

The power of the (collaborating) crowd
optimizing graduate student descent



COMMUNICATION AND REUSE



You can

1. Participate in upcoming RAMPs
2. Use RAMP in teaching or training
3. Use the toolkit for your own workflows
4. Submit it to us if you want to run a data challenge

LINKS

frontend:

www.ramp.studio

toolkit:

github.com/paris-saclay-cds/ramp-workflow

examples:

github.com/ramp-kits

slack:

ramp-studio.slack.com

READING MATERIAL

- **medium.com/@balazskegl**
  - The data science ecosystem (industrial edition)
  - Teaching the data science process
  - How to build a data science pipeline
- **RAMP paper**
  - https://openreview.net/forum?id=Syg4NHz4eQ