

RAMP DATA CHALLENGES WITH MODULARIZATION AND CODE SUBMISSION *LESSONS LEARNED*

BALÁzs KÉGL

Université Paris-Saclay / CNRS

WHO AM I?

Balázs Kégl

- Directeur de recherche **CNRS**
 - machine learning (20 years)
interfacing with particle physics (10 years)
- Director of the **Paris-Saclay Center for Data Science**
 - interfacing with biology, economy, climatology, chemistry, etc. (4 years)
- Data science **consulting and training** (4 years)

OUTLINE

- A **short history** of RAMPs
 - **motivations, design principles, and the current tool**
- Three data challenges
 - **anomaly detection** in the LHC ATLAS detector
 - **classifying** and **quantifying** drug preparations for cancer therapy
 - **time series forecasting** of El Niño
- How can **you use it?**
 - in a **classroom**: to **teach ML**
 - as a **domain scientist**: to **crowdsource your predictive problem**
 - as a **data scientist**: to **benchmark your new techniques**

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, 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

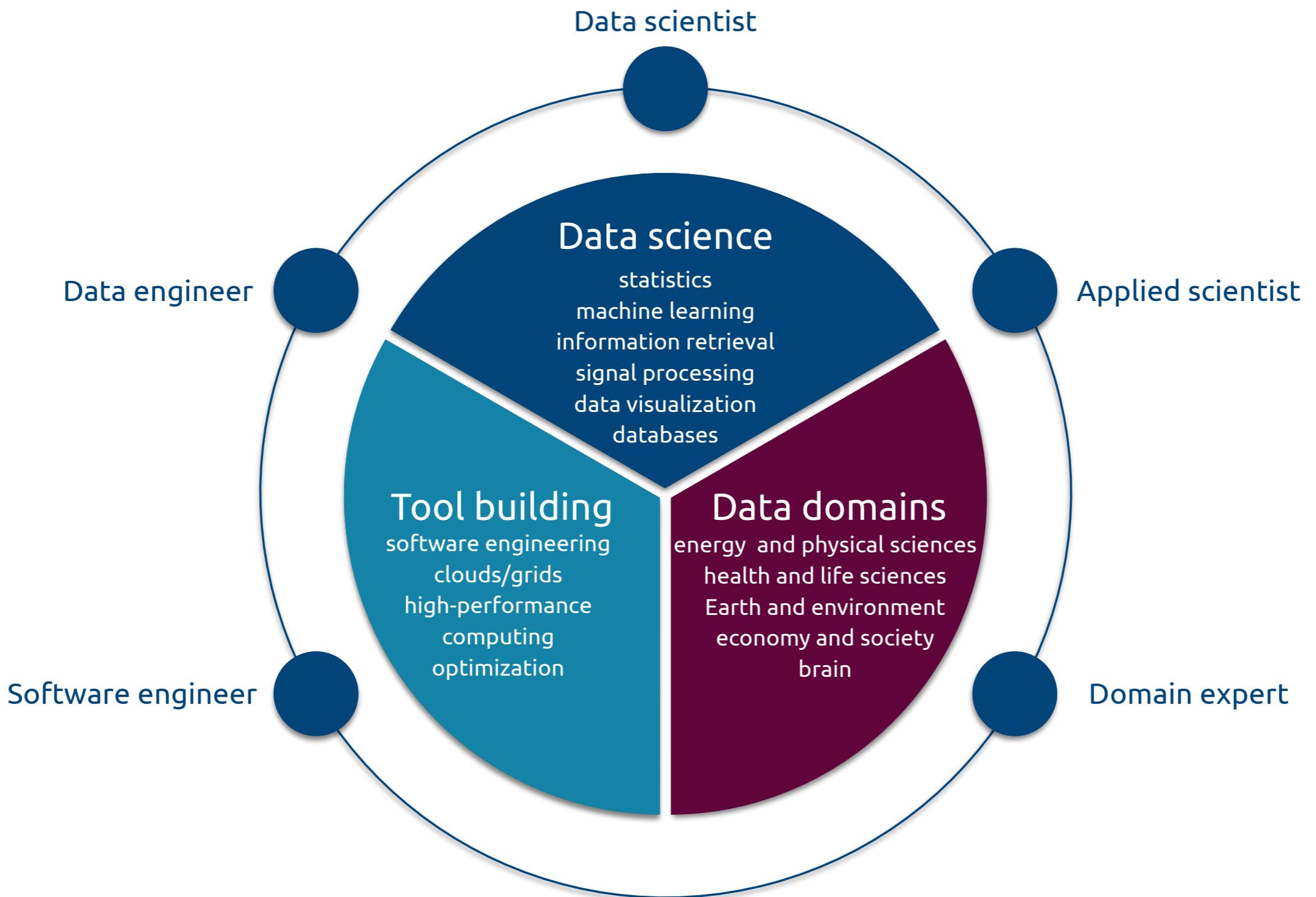
LTCI/Telecom
CMA/Polytechnique
CVN/Centrale
LSS/Supélec
CMLA/Cachan
LIMSI
DTIM/ONERA

Statistics

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

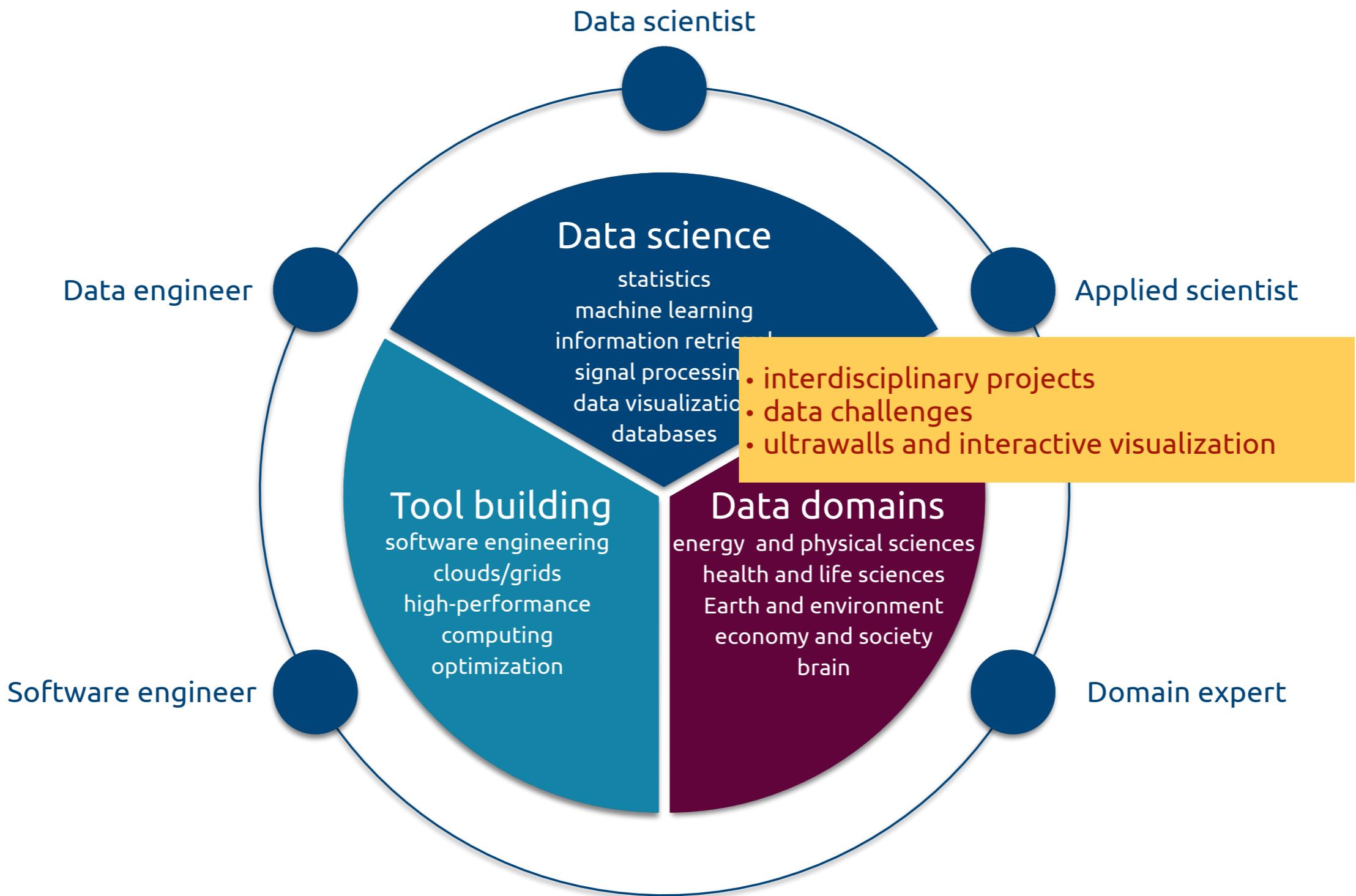
THE DATA SCIENCE ECOSYSTEM

<https://medium.com/@balazskegl>



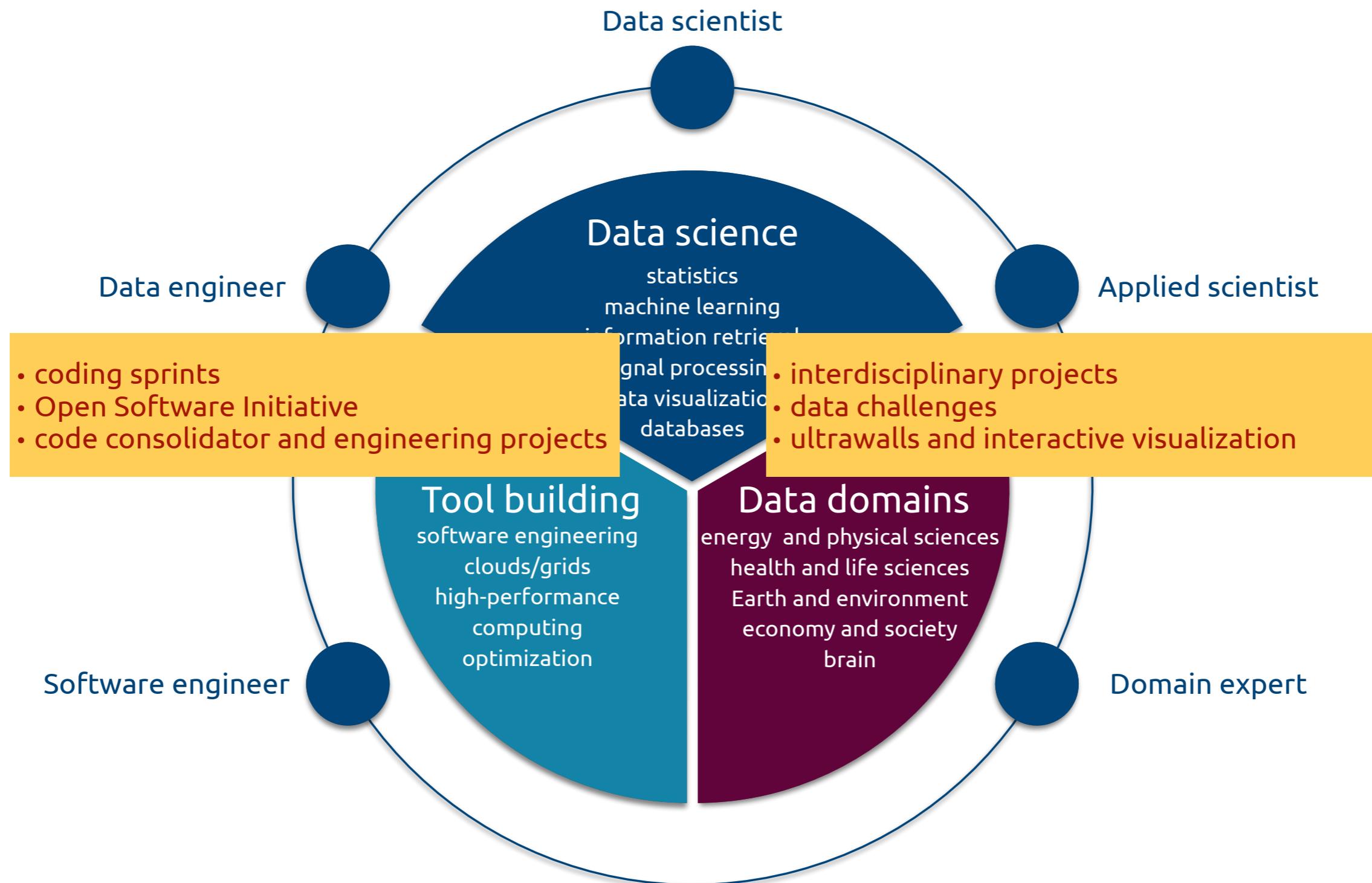
THE DATA SCIENCE ECOSYSTEM

<https://medium.com/@balazskegl>



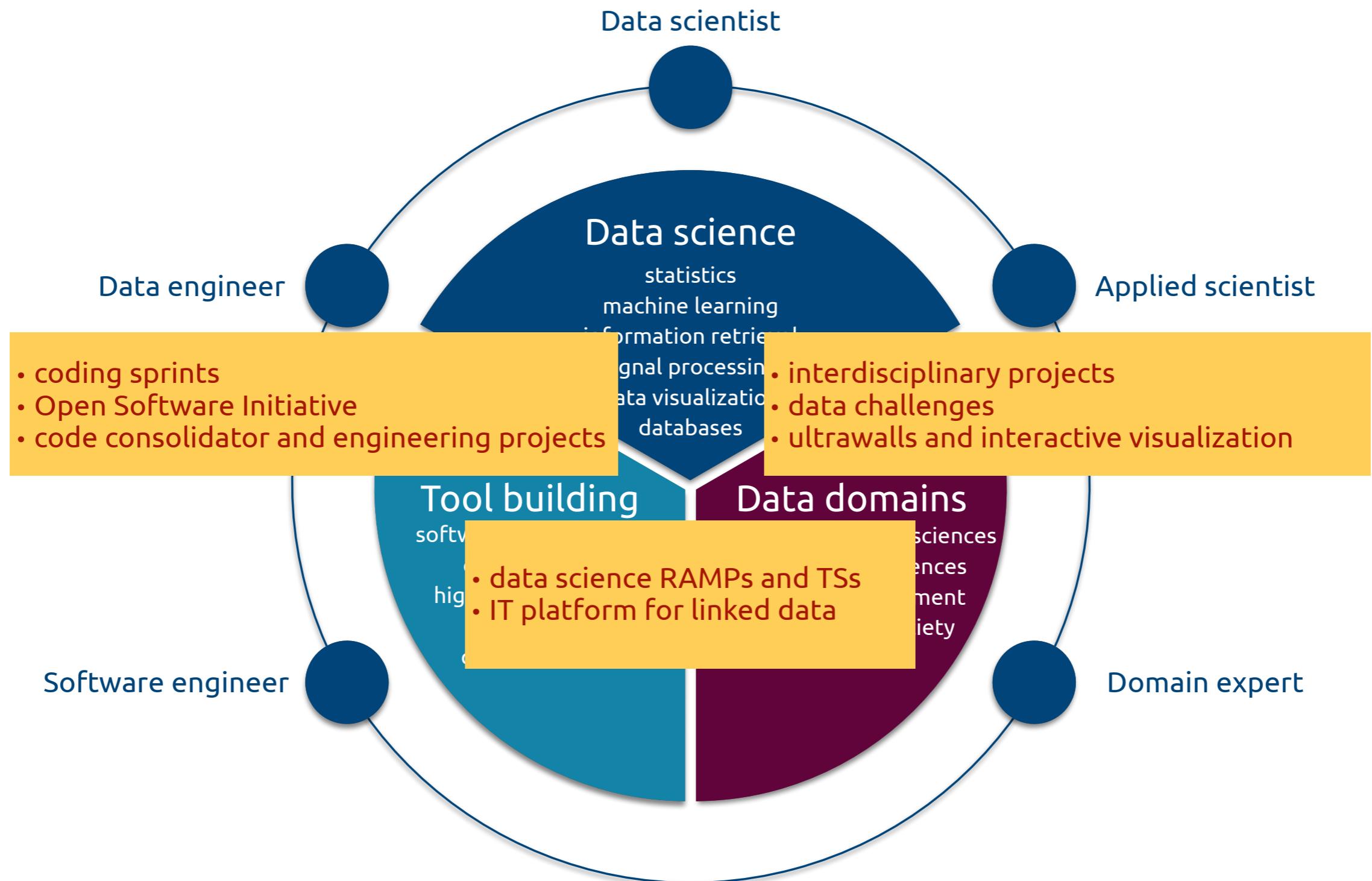
THE DATA SCIENCE ECOSYSTEM

<https://medium.com/@balazskegl>



THE DATA SCIENCE ECOSYSTEM

<https://medium.com/@balazskegl>



LACK OF TOOLS

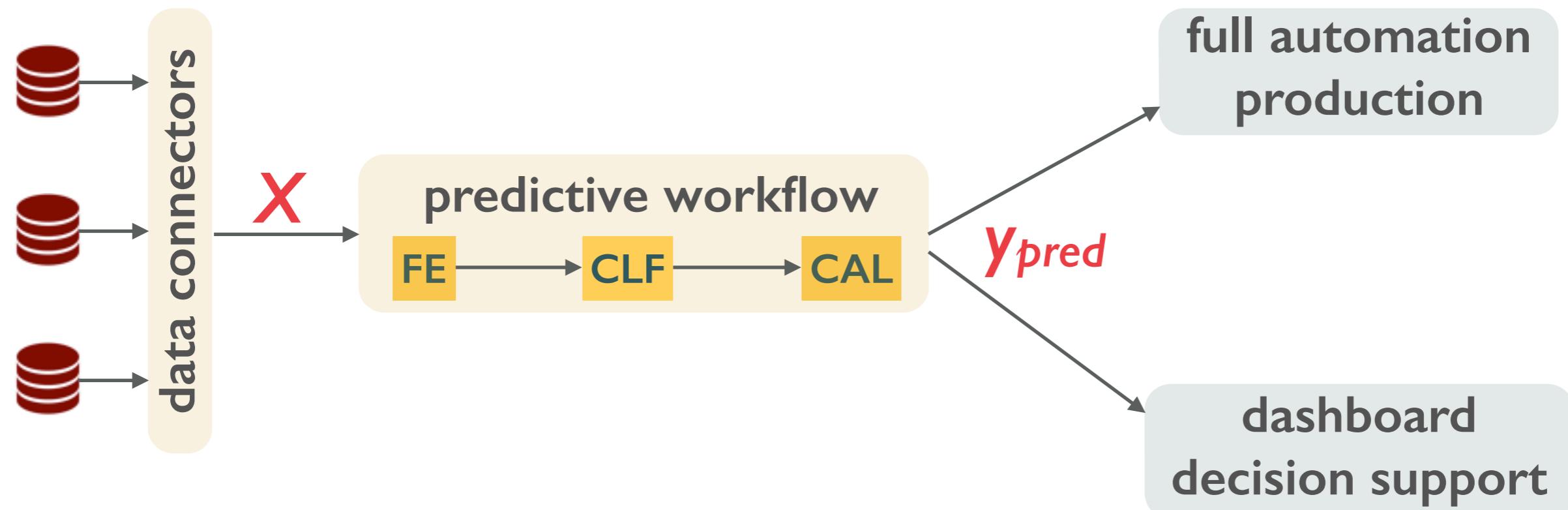
- We have realized how much **data scientists are ill-equipped to manage the data science development process**
 - collaborating with domain scientists or business units on data-driven problem/product formulation
 - bench for logging experiments, guiding (human) model search and tuning
 - managing data science teams and collaborating with each other
 - collaborating with AI (out-of-the-box AutoML does not work: the search space is too big)
 - managing the **productionalization** of a prototype model

GOAL

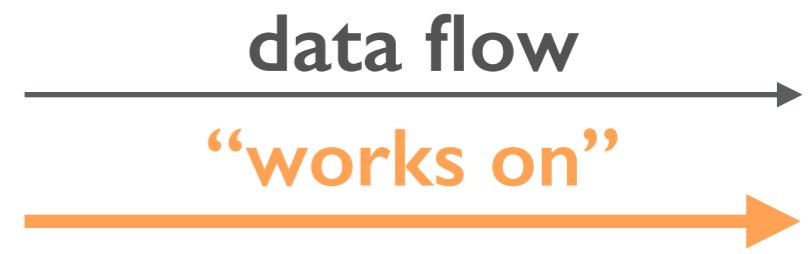
- Design a **data science pipeline development** tool that
 - **hides heavy computational details** and provides a **simple interface** to data scientists to **experiment with algorithms**
 - promotes **collaboration** and the rapid **propagation of ideas**
 - **modularizes complex pipelines** so the different expertise can be applied without having to understand all the details of the full workflow
 - allows the challenge organizer to walk away with a **working prototype**

THE DATA FLOW

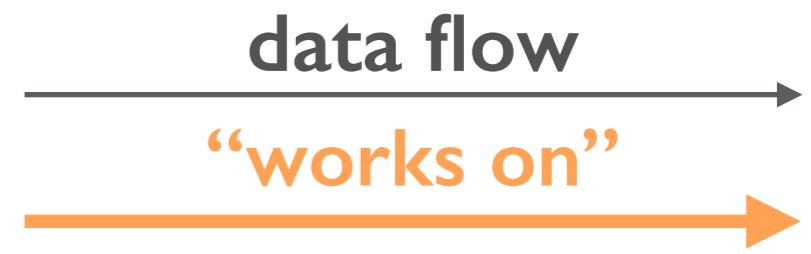
data flow →



THE IDEAL SEQUENCE

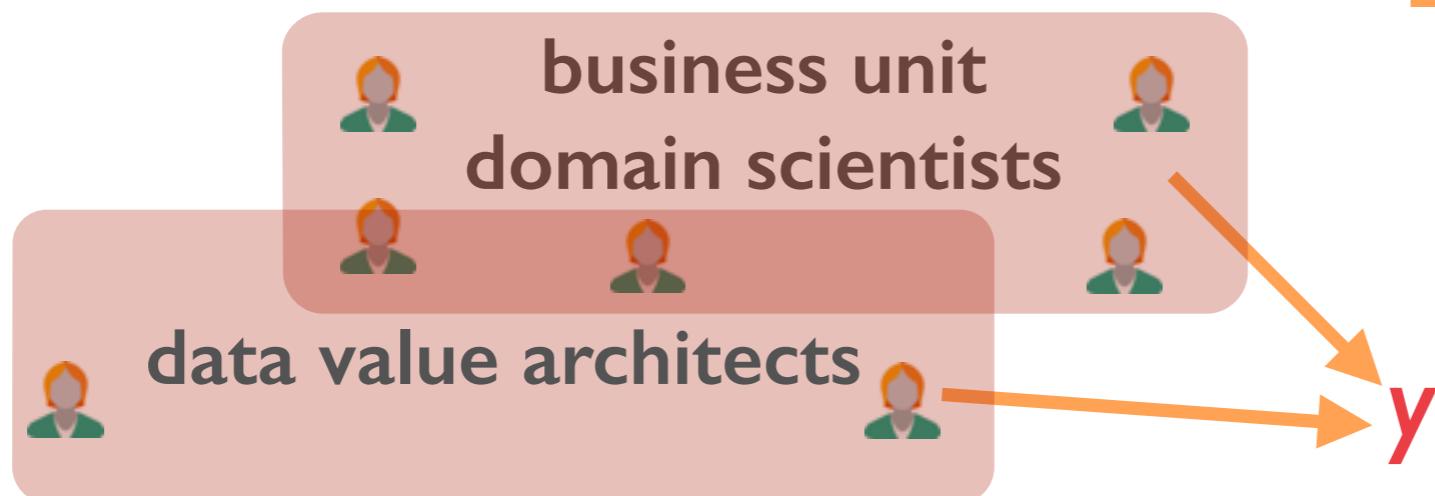


THE IDEAL SEQUENCE

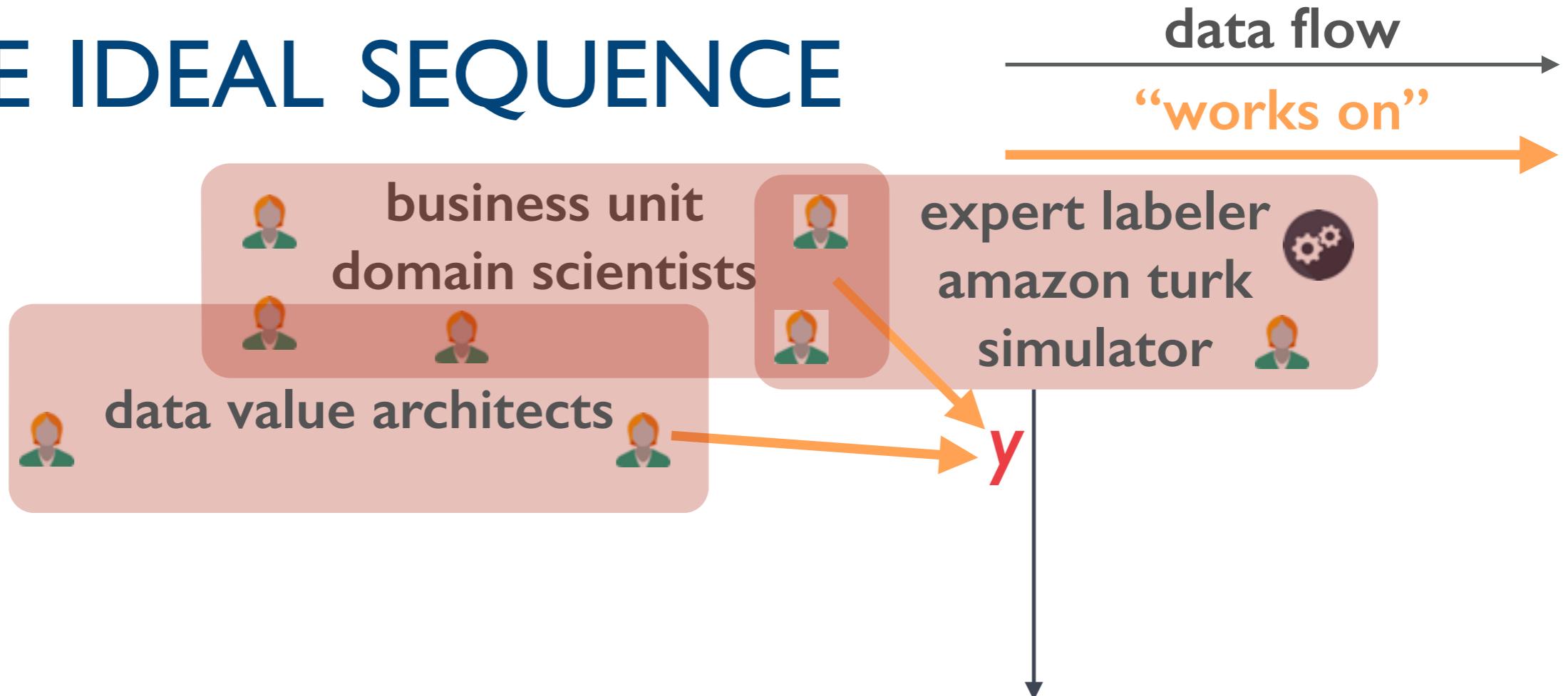


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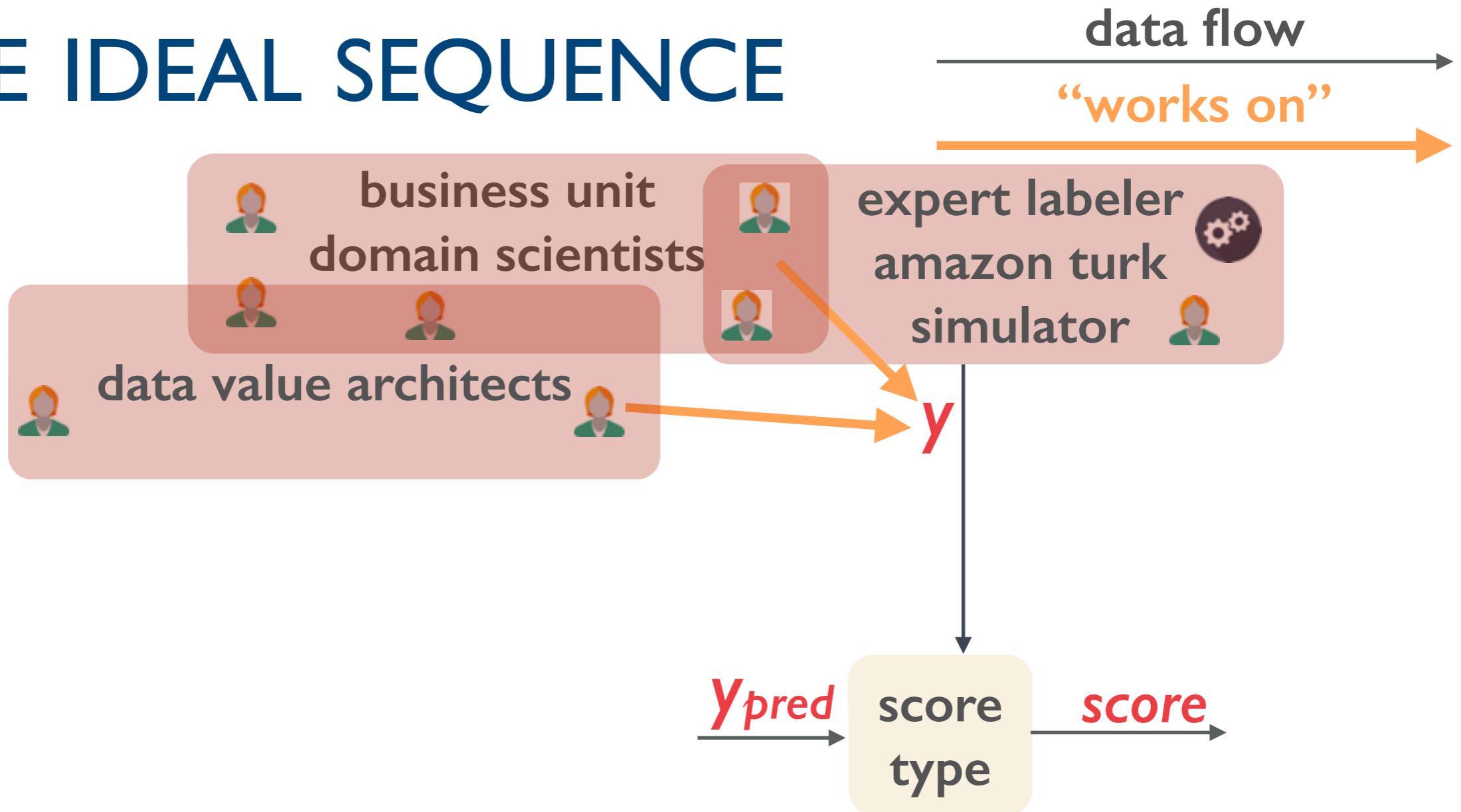
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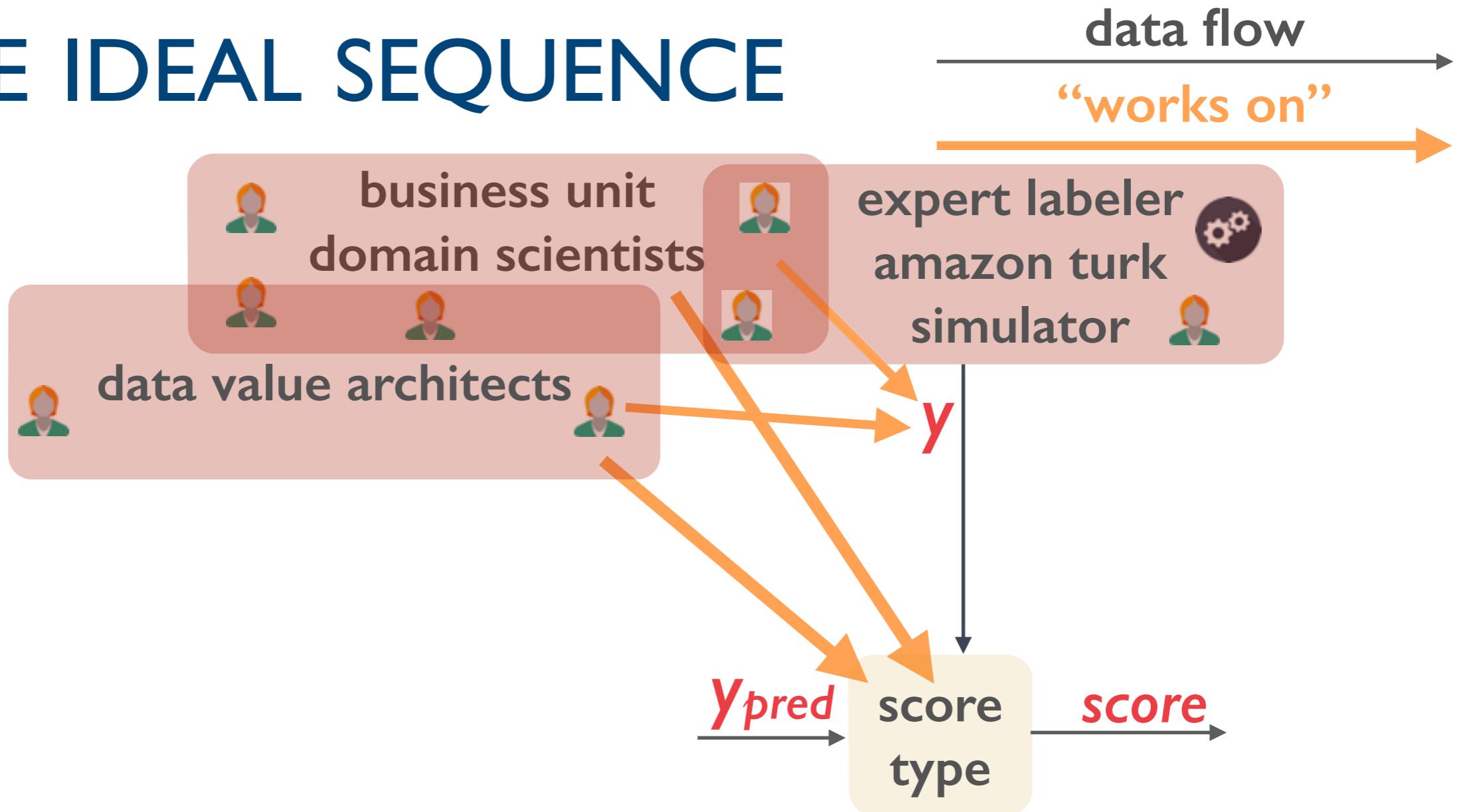
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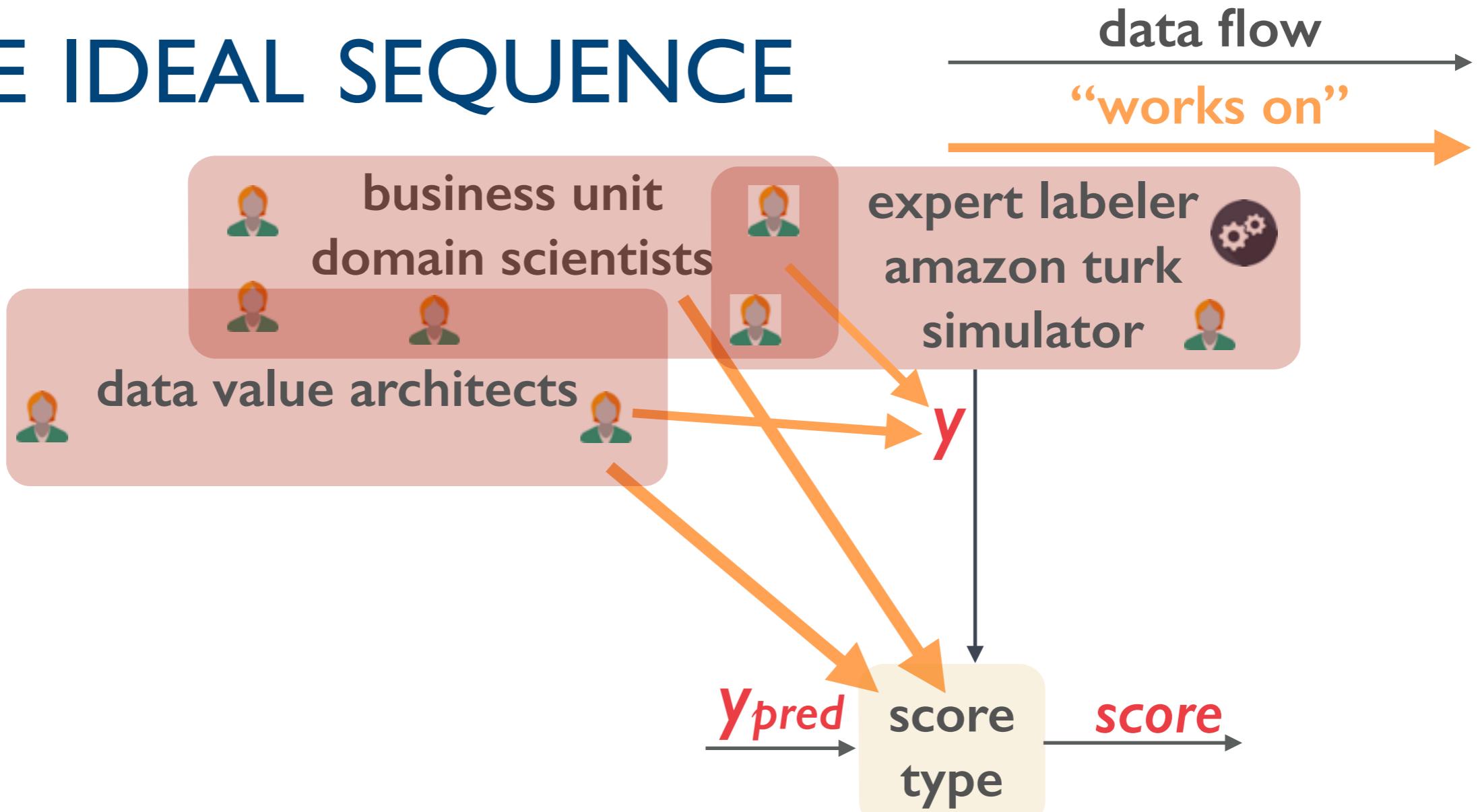
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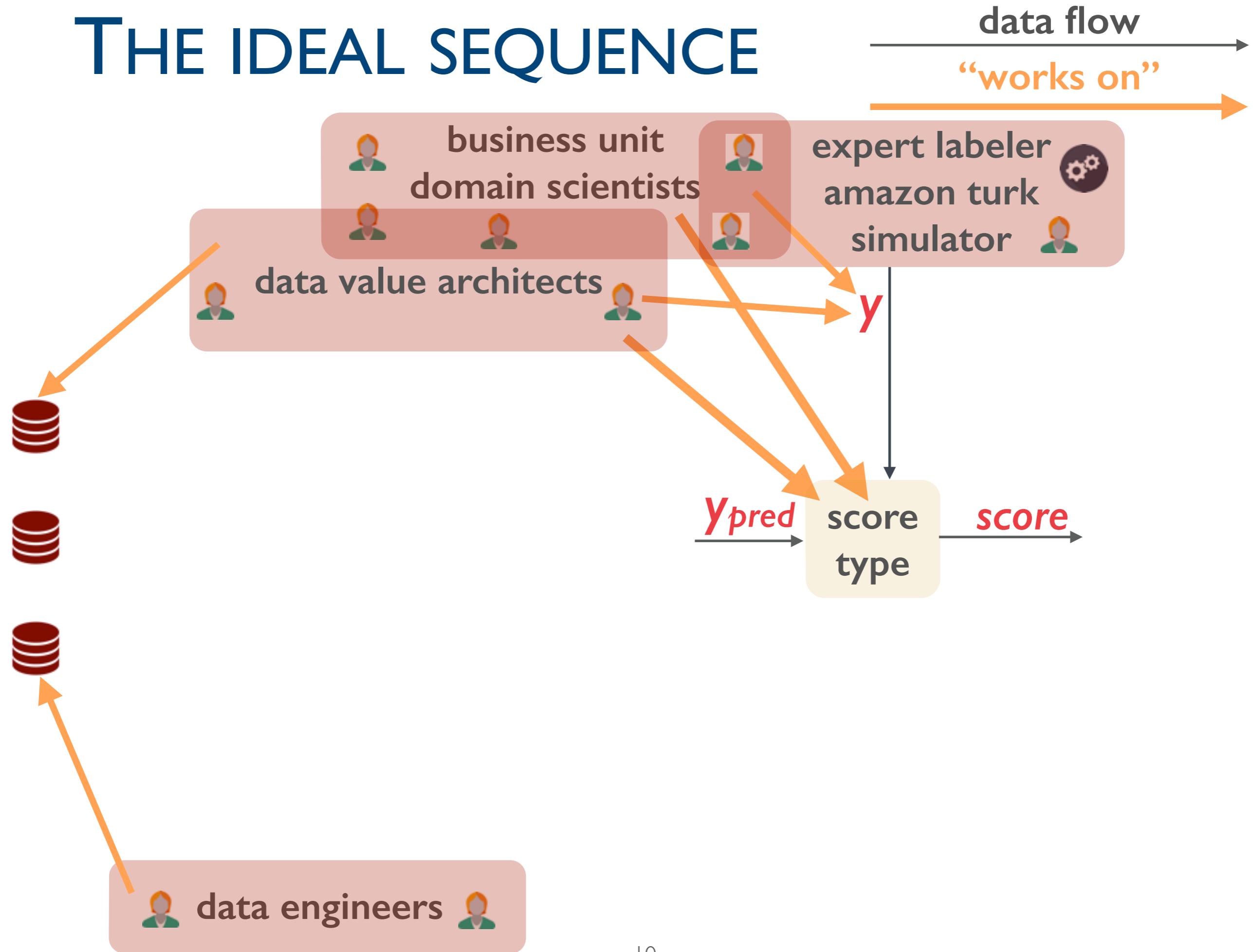
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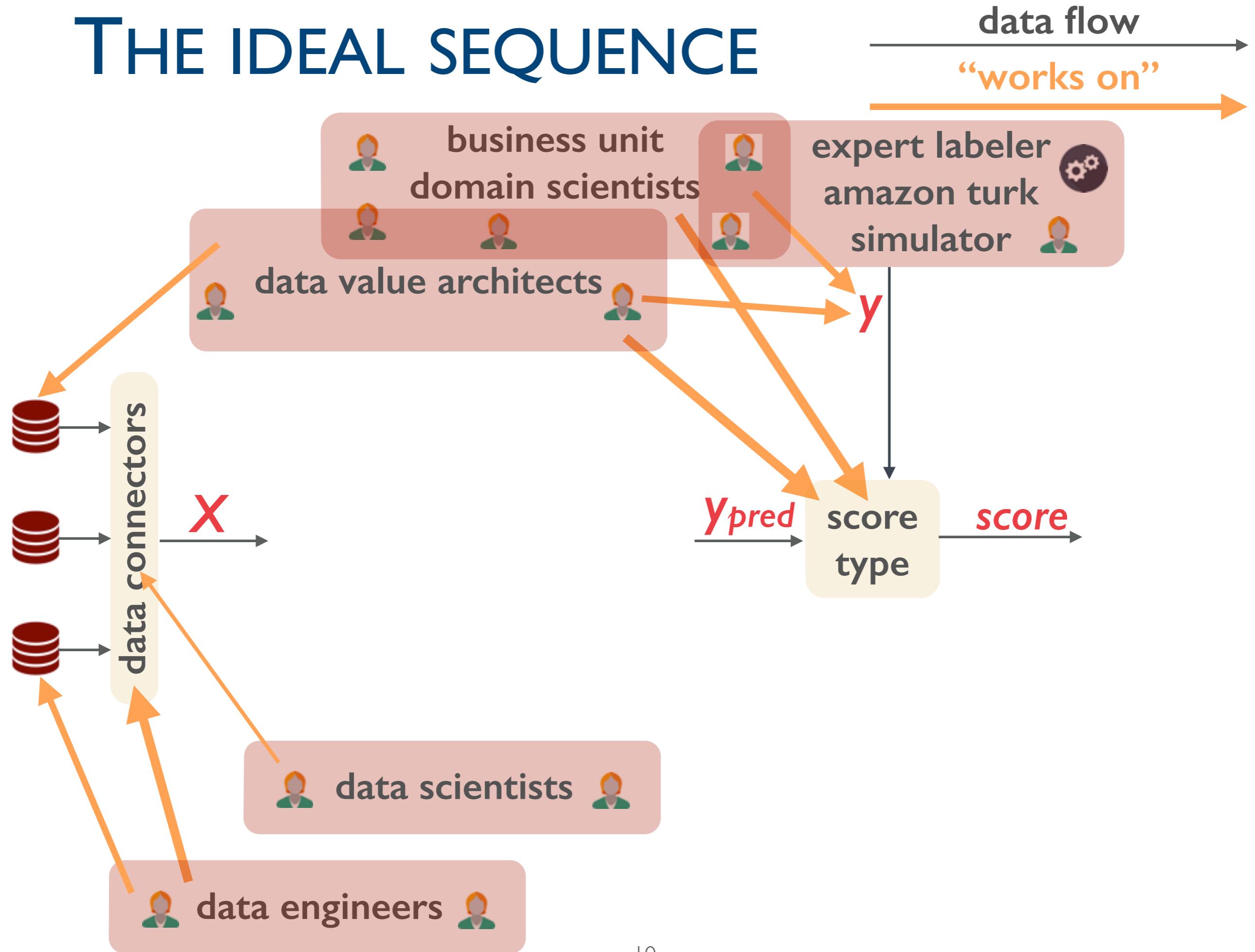
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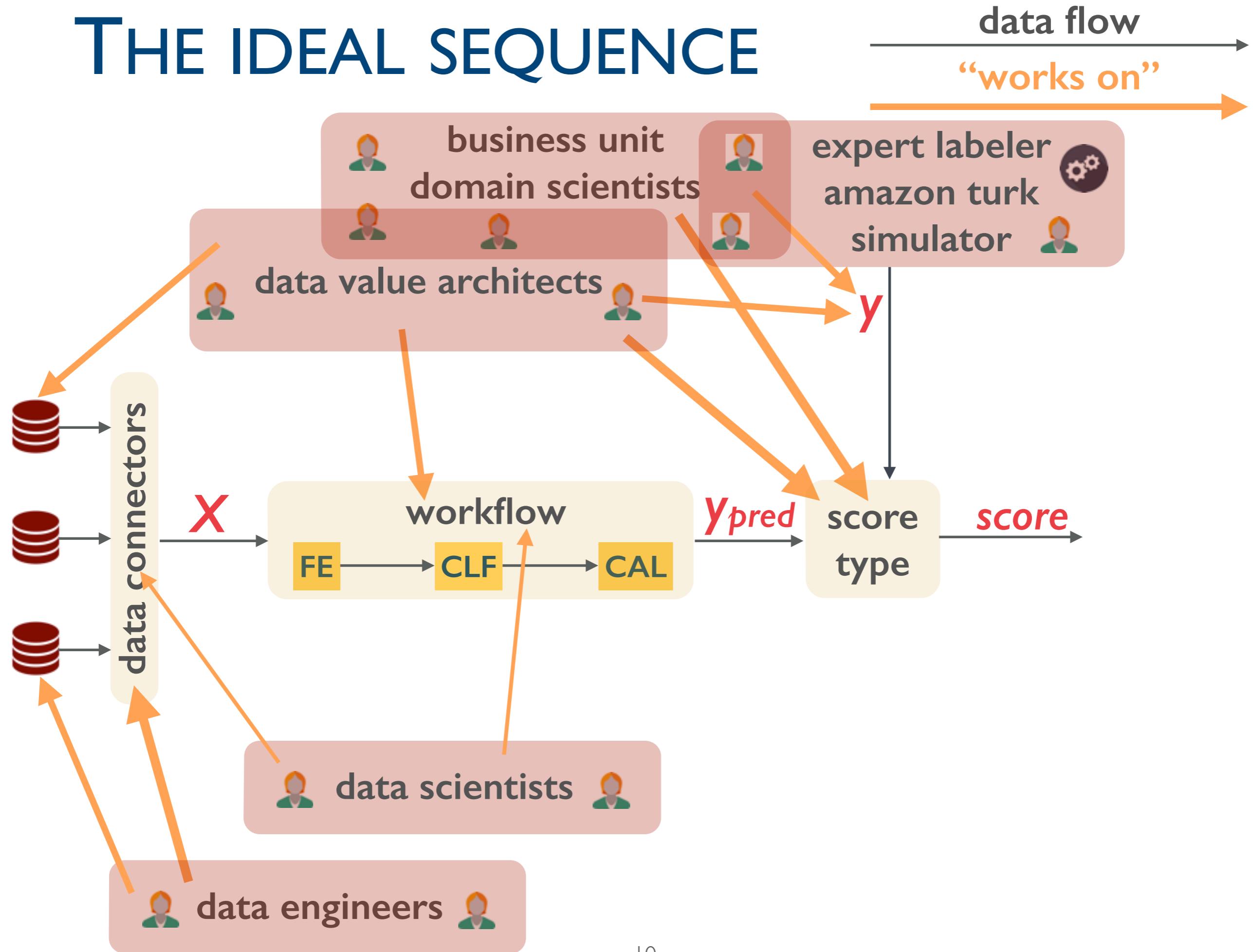
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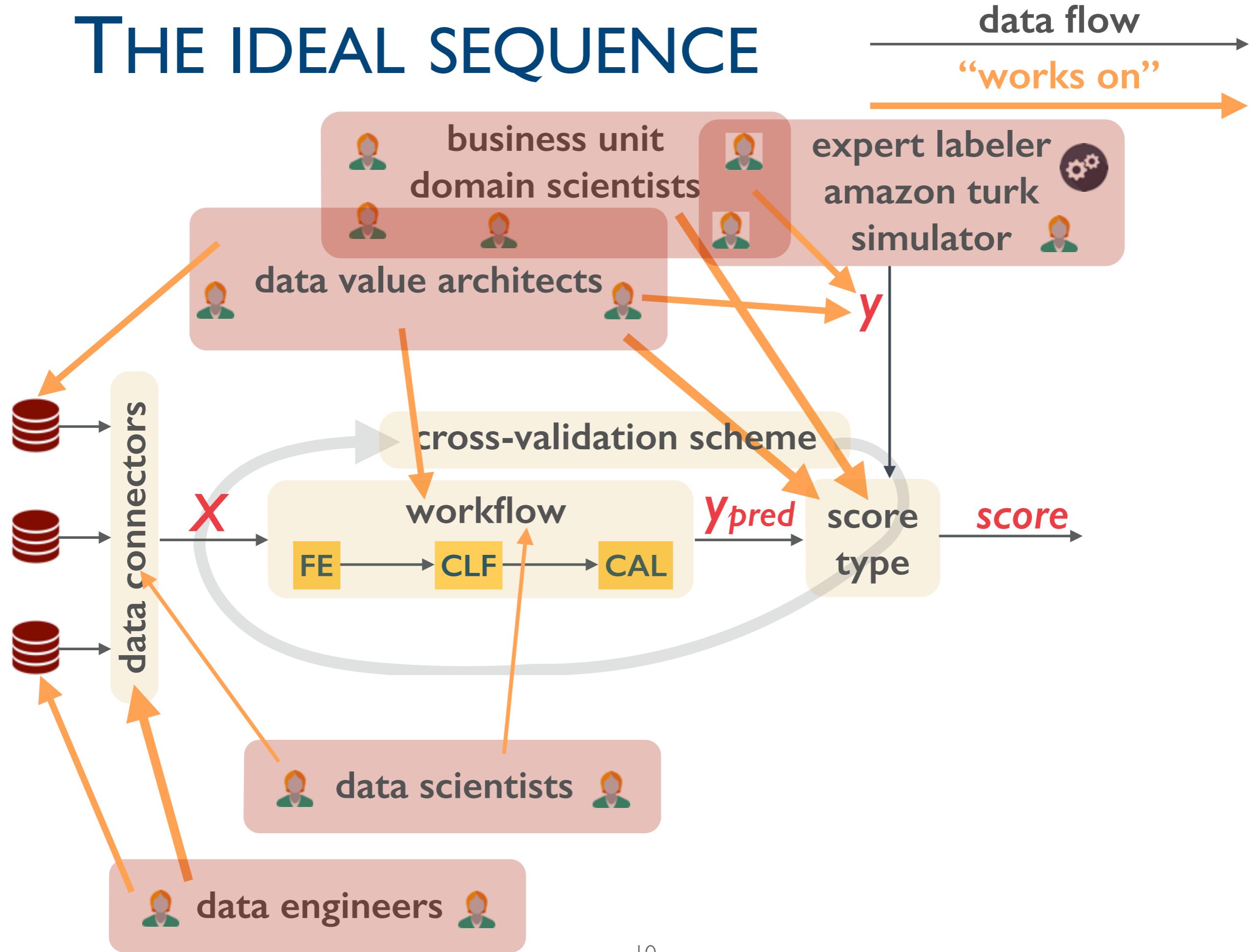
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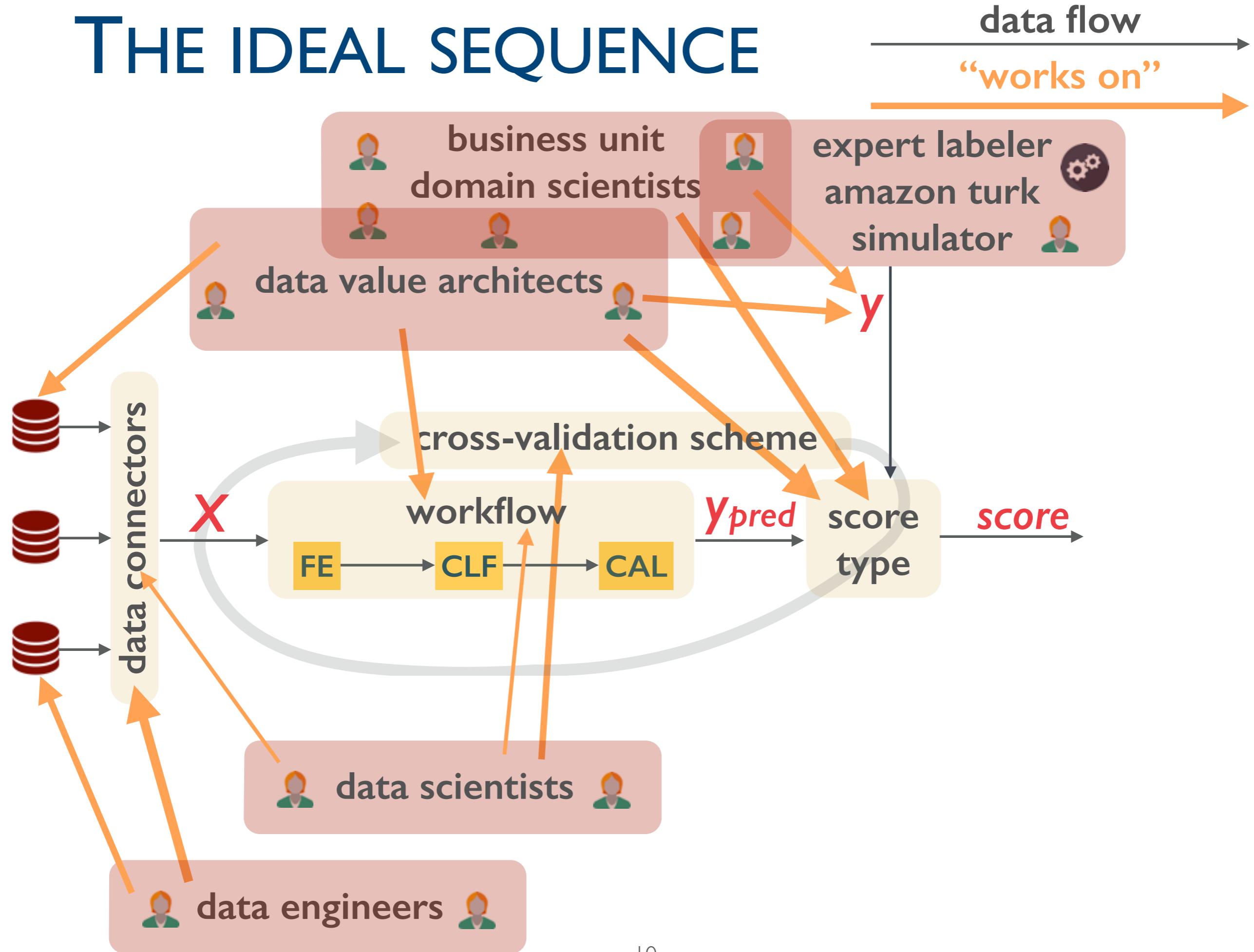
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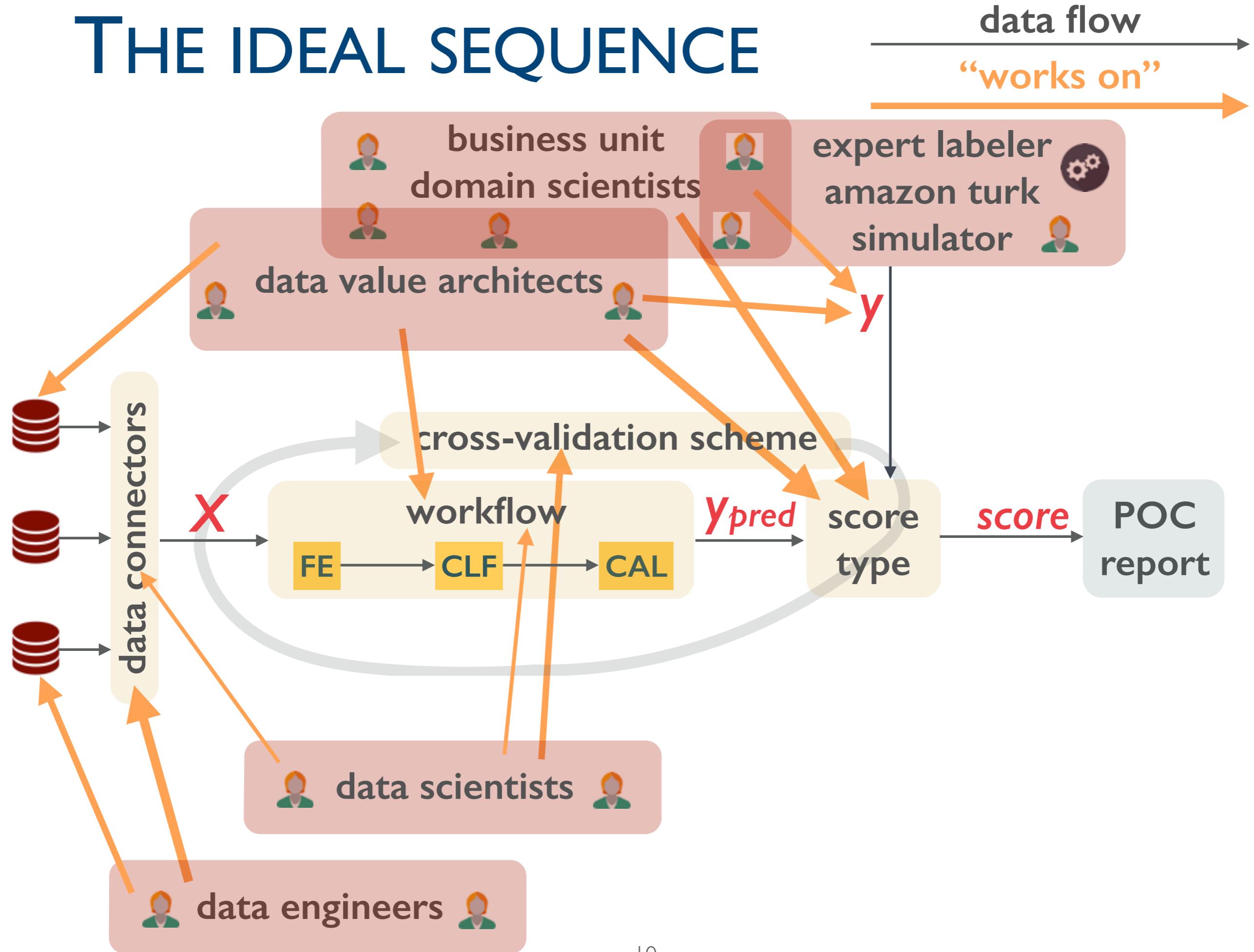
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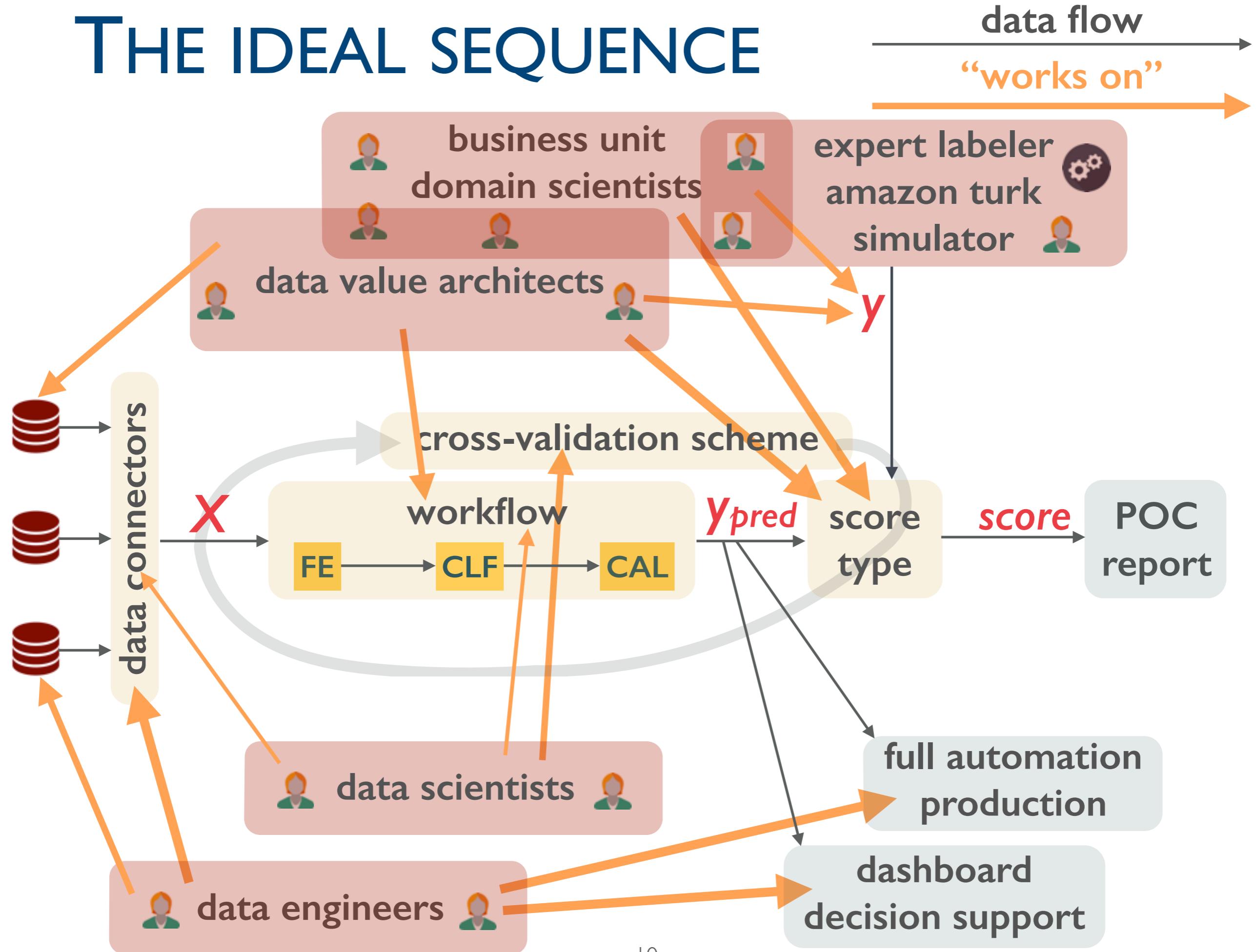
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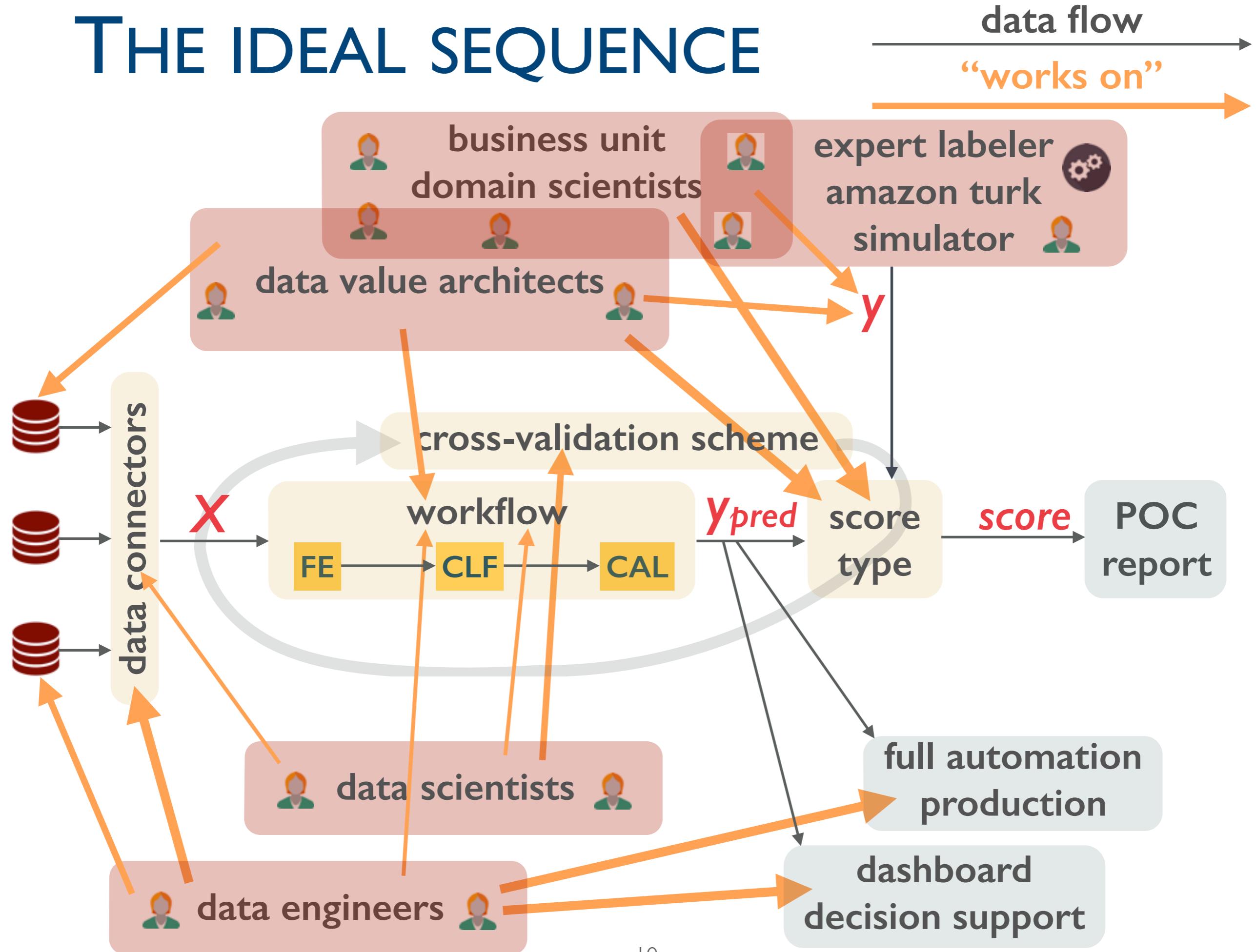
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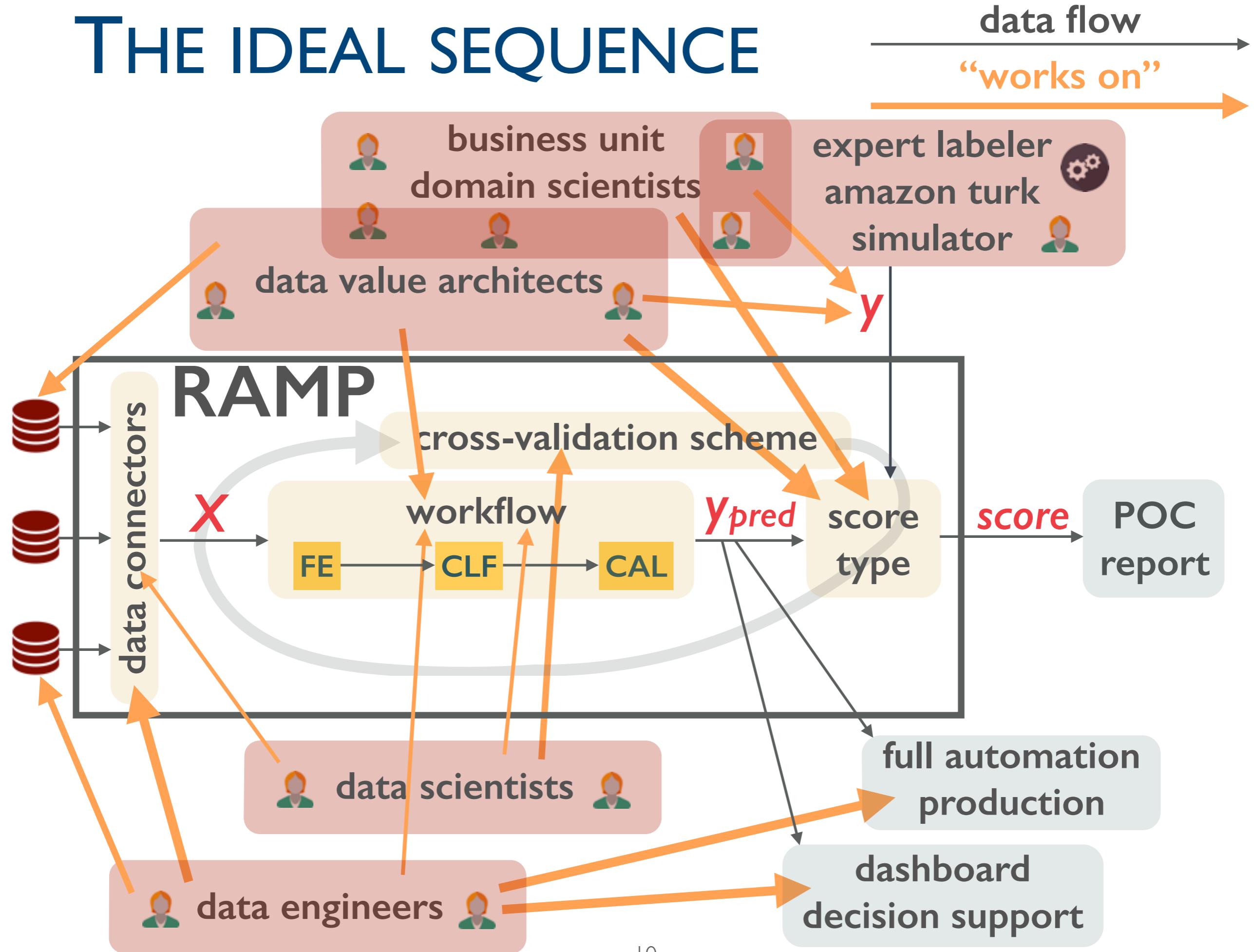
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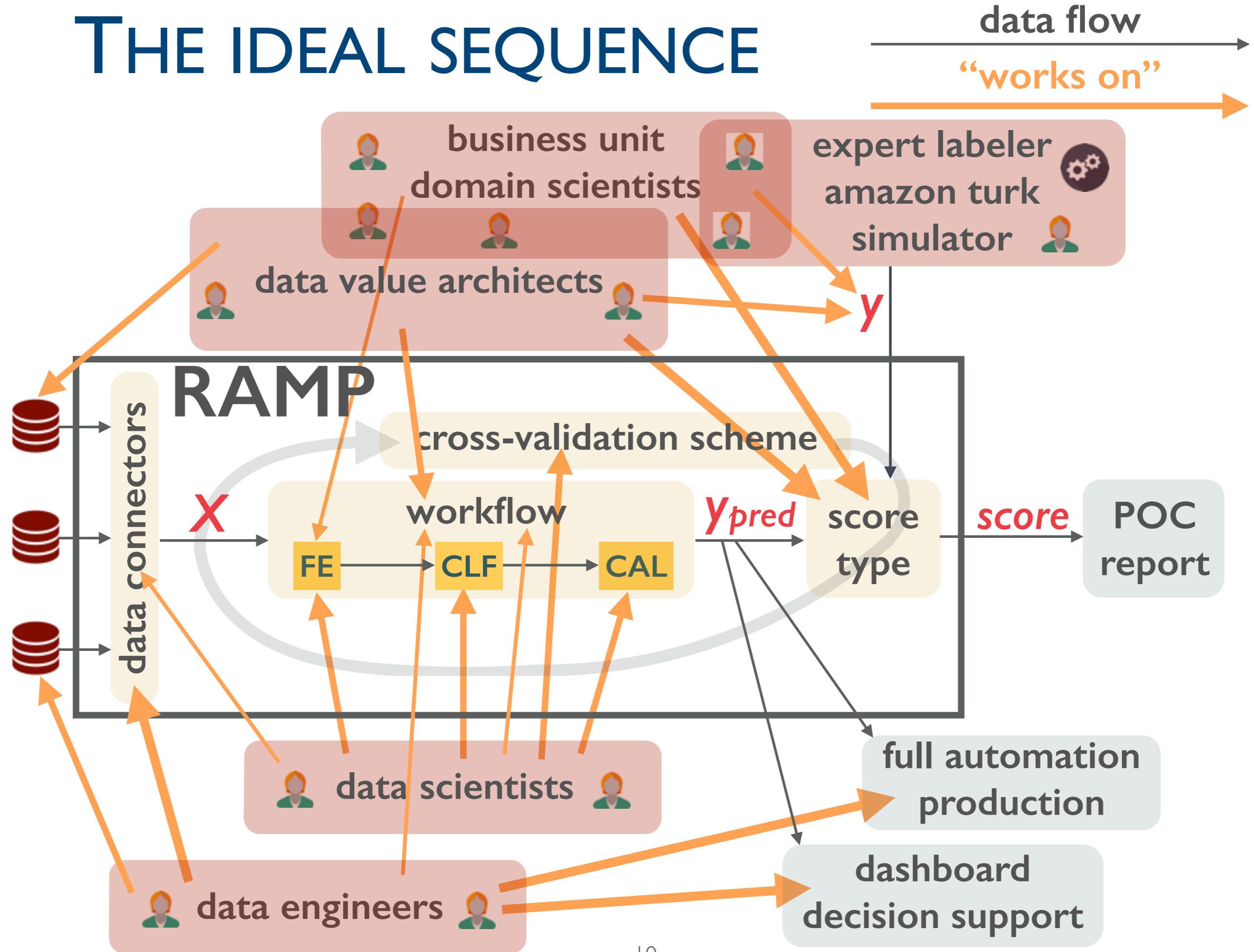
THE IDEAL SEQUENCE



THE IDEAL SEQUENCE

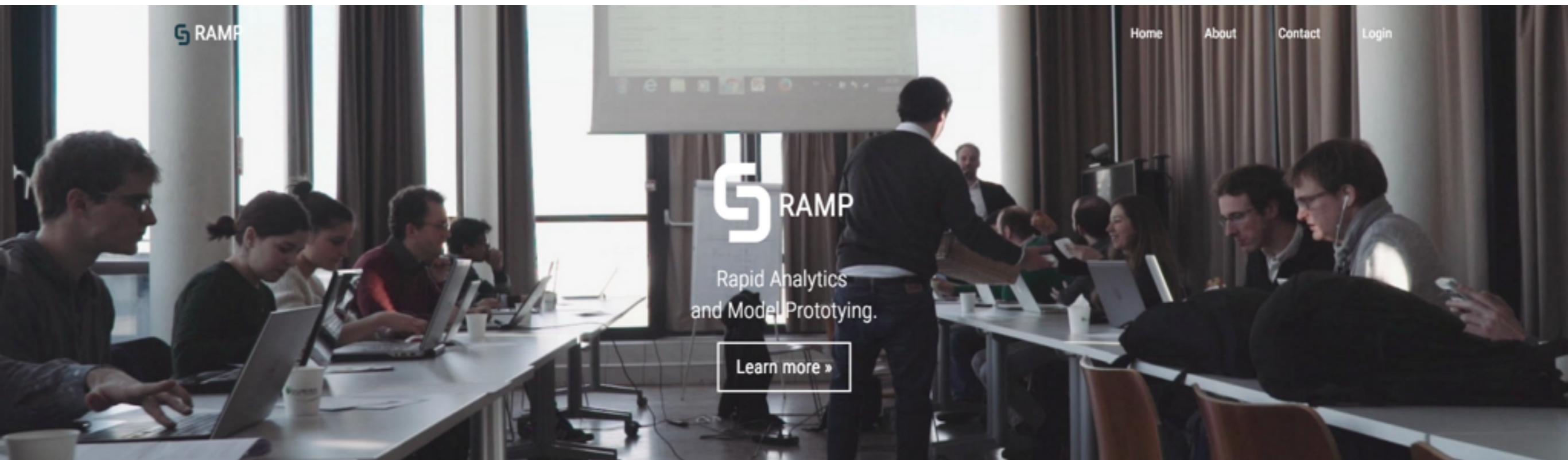


THE IDEAL SEQUENCE



RAPID ANALYTICS AND MODEL PROTOTYPING (RAMP)

<http://www.ramp.studio>



Collaborative prototyping

During the RAMP, the participants submit predictive solutions (code). The models are trained on our back-end. The scores are displayed on a leaderboard. All participants have access to all code, and they are encouraged to look at and to reuse each other's solutions. This accelerates the development process since good ideas spread fast.



Training

A great tool to learn data science! RAMPs are used in the MS Big Data at Telecom ParisTech, in three UPSaclay M2 programs (Data Science, AIC, Data and Knowledge), in a course on Machine Learning for Finance and Economics at Université Panthéon-Assas, in a graduate course in the Data analysis and decision program at Ecole Centrale de Lille.



Networking

Each RAMP attracts about 30-50 participants, coming from different backgrounds and career stages, who usually meet for the first time. They develop a working relationship in a relaxed environment, and sometimes keep working together after the event.

RAPID ANALYTICS AND MODEL PROTOTYPING (RAMP)

<http://www.ramp.studio>

Team



Balázs Kégl



Alex Gramfort



Akin Kazakçı



Mehdi Cherti



Yohann Sitruk

Alumni



Djalel Benbouzid



Camille Marini

RAMP

RAPID ANALYTICS AND MODEL PROTOTYPING

- Roughly two formats
 - single day hackatons with 20-50 participants, open leaderboard, 15 minute timeout
 - 1-3 week classroom challenges up 150 students (but no limit really): closed phase followed by an open phase
- 800+ users, 5000+ predictive models

CURRENT RAMPs

www.ramp.studio/problems

RAMP

Hi Balazs! ▾

- **Pollinating insect classification (209 classes)**
 - La Paillasse / Futur en Seine, number of participants = **28**, number of submissions = **13**, combined score = **0.831**, [click here for score vs time plot](#)
- **Titanic survival classification**
 - DSSP 6 2016/17 2, number of participants = **31**, number of submissions = **34**, combined score = **0.87**, [click here for score vs time plot](#)
 - Entry exam to deep learning tutorial, number of participants = **35**, number of submissions = **21**, combined score = **0.86**, [click here for score vs time plot](#)
 - Ecole des Mines 2016/17, number of participants = **125**, number of submissions = **144**, combined score = **0.89**, [click here for score vs time plot](#)
- **Pollinating insect classification (18 classes)**
 - Polytechnique MAP583/MAP542 2016/17, number of participants = **166**, number of submissions = **114**, combined score = **0.959**, [click here for score vs time plot](#)
 - DSSP5 2017, number of participants = **15**, number of submissions = **24**, combined score = **0.93**, [click here for score vs time plot](#)
- **Particle tracking in the LHC ATLAS detector**
 - initial single-day RAMP 2017, number of participants = **55**, number of submissions = **60**, combined score = **0.97**, [click here for score vs time plot](#)
- **El Nino forecast**
 - single-day RAMP at Climate Informatics Workshop 2015; Saclay Data Camp 2016/17, number of participants = **160**, number of submissions = **138**, combined score = **0.389**, [click here for score vs time plot](#)
- **Arctic sea ice forecast**
 - single-day RAMP at Climate Informatics Workshop 2016, number of participants = **46**, number of submissions = **83**, combined score = **0.31**, [click here for score vs time plot](#)
 - Polytechnique MAP542 2016/17, number of participants = **20**, number of submissions = **52**, combined score = **0.268**, [click here for score vs time plot](#)
 - Polytechnique MAP583 2016/17, number of participants = **123**, number of submissions = **252**, combined score = **0.259**, [click here for score vs time plot](#)
- **Number of air passengers prediction**
 - DSSP4/5 2016, number of participants = **95**, number of submissions = **242**, combined score = **0.236**, [click here for score vs time plot](#)
 - DSSP6 2017, number of participants = **23**, number of submissions = **59**, combined score = **0.268**, [click here for score vs time plot](#)
- **Drug classification and concentration estimation from Raman spectra**
 - Polytechnique MAP583 2016/17, number of participants = **125**, number of submissions = **258**, combined score = **0.048**, [click here for score vs time plot](#)
 - initial single-day RAMP 2016; Saclay Data Camp 2016/17, number of participants = **242**, number of submissions = **554**, combined score = **0.027**, [click here for score vs time plot](#)
 - Ecole des Mines 2016/17, number of participants = **124**, number of submissions = **560**, combined score = **0.023**, [click here for score vs time plot](#)
- **Detecting anomalies in the LHC ATLAS detector**
 - Polytechnique MAP542 2016/17, number of participants = **29**, number of submissions = **47**, combined score = **0.865**, [click here for score vs time plot](#)
 - Polytechnique MAP583 2016/17, number of participants = **133**, number of submissions = **275**, combined score = **0.899**, [click here for score vs time plot](#)
 - initial single-day RAMP 2016, number of participants = **49**, number of submissions = **19**, combined score = **0.677**, [click here for score vs time plot](#)
- **Epidemium cancer mortality rate prediction (2nd RAMP)**
 - initial single-day RAMP 2016, number of participants = **39**, number of submissions = **46**, combined score = **21.79**, [click here for score vs time plot](#)
 - Polytechnique MAP583 2016/17, number of participants = **128**, number of submissions = **192**, combined score = **18.59**, [click here for score vs time plot](#)
 - Polytechnique MAP542 2016/17, number of participants = **22**, number of submissions = **57**, combined score = **19.31**, [click here for score vs time plot](#)

DATA SCIENCE THEMES

C ⌂ ⓘ www.ramp.studio/data_science_themes

☰ RAMP

Data science themes

• classification

- Iris classification
- Detecting anomalies in the LHC ATLAS detector
- Drug classification and concentration estimation from Raman spectra
- Titanic survival classification
- Pollenating insect classification (18 classes)
- Pollenating insect classification (209 classes)

• convolutional networks

- Pollenating insect classification (18 classes)
- Pollenating insect classification (209 classes)

• external data

- Number of air passengers prediction

• feature engineering

- El Nino forecast
- Arctic sea ice forecast
- Drug classification and concentration estimation from Raman spectra
- Detecting anomalies in the LHC ATLAS detector

• forests

- Iris classification
- Detecting anomalies in the LHC ATLAS detector
- Titanic survival classification
- Boston housing price regression
- El Nino forecast
- Arctic sea ice forecast
- Number of air passengers prediction
- Epidemium cancer mortality rate prediction (2nd RAMP)

• functional data

- Drug classification and concentration estimation from Raman spectra

• image data

- Pollenating insect classification (18 classes)
- Pollenating insect classification (209 classes)
- El Nino forecast

⌂ ⓘ www.ramp.studio/data_science_themes

☰ RAMP

• missing data

- Epidemium cancer mortality rate prediction (2nd RAMP)
- Titanic survival classification

• neural networks (deep learning)

- Drug classification and concentration estimation from Raman spectra
- Pollenating insect classification (18 classes)
- Pollenating insect classification (209 classes)

• regression

- Boston housing price regression
- El Nino forecast
- Arctic sea ice forecast
- Number of air passengers prediction
- Drug classification and concentration estimation from Raman spectra
- Epidemium cancer mortality rate prediction (2nd RAMP)

• small data

- Drug classification and concentration estimation from Raman spectra
- Epidemium cancer mortality rate prediction (2nd RAMP)
- Detecting anomalies in the LHC ATLAS detector
- El Nino forecast
- Arctic sea ice forecast
- Number of air passengers prediction
- Particle tracking in the LHC ATLAS detector

• supervised clustering (unsupervised classification)

- Particle tracking in the LHC ATLAS detector

• tabular data

- Iris classification
- Detecting anomalies in the LHC ATLAS detector
- Titanic survival classification
- Boston housing price regression
- Number of air passengers prediction
- Epidemium cancer mortality rate prediction (2nd RAMP)

• time series forecasting

- El Nino forecast
- Arctic sea ice forecast

DATA DOMAINS

The screenshot shows a web browser displaying the RAMP (Research and Application of Machine Learning) website at www.ramp.studio/data_domains. The page has a dark theme with a teal header bar. On the left, there is a sidebar with icons for users, help, and a question mark. The main content area is titled "RAMP" and contains two sections: "Industrial data domains" and "Scientific data domains".

Industrial data domains

- **travel**
 - Number of air passengers prediction

Scientific data domains

- **climate science**
 - El Nino forecast
 - Arctic sea ice forecast
- **ecology**
 - Pollenating insect classification (18 classes)
 - Pollenating insect classification (209 classes)
- **healthcare**
 - Drug classification and concentration estimation from Raman spectra
 - Epidemium cancer mortality rate prediction (2nd RAMP)
- **particle physics**
 - Detecting anomalies in the LHC ATLAS detector
 - Particle tracking in the LHC ATLAS detector

RAMP

DATA CHALLENGE WITH *CODE SUBMISSION*

frontend



backend



data

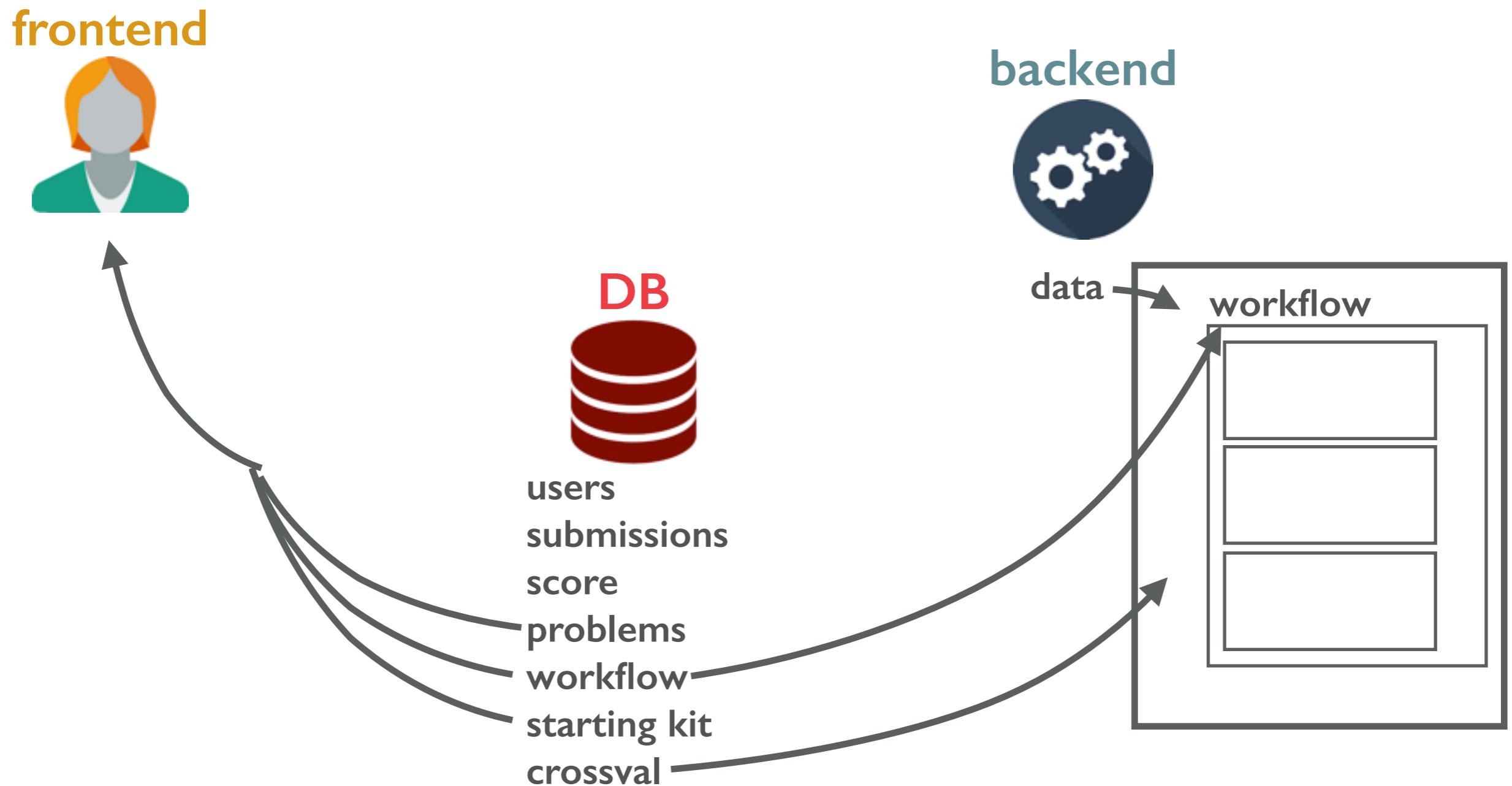
DB



users
submissions
score
problems
workflow
starting kit
crossval

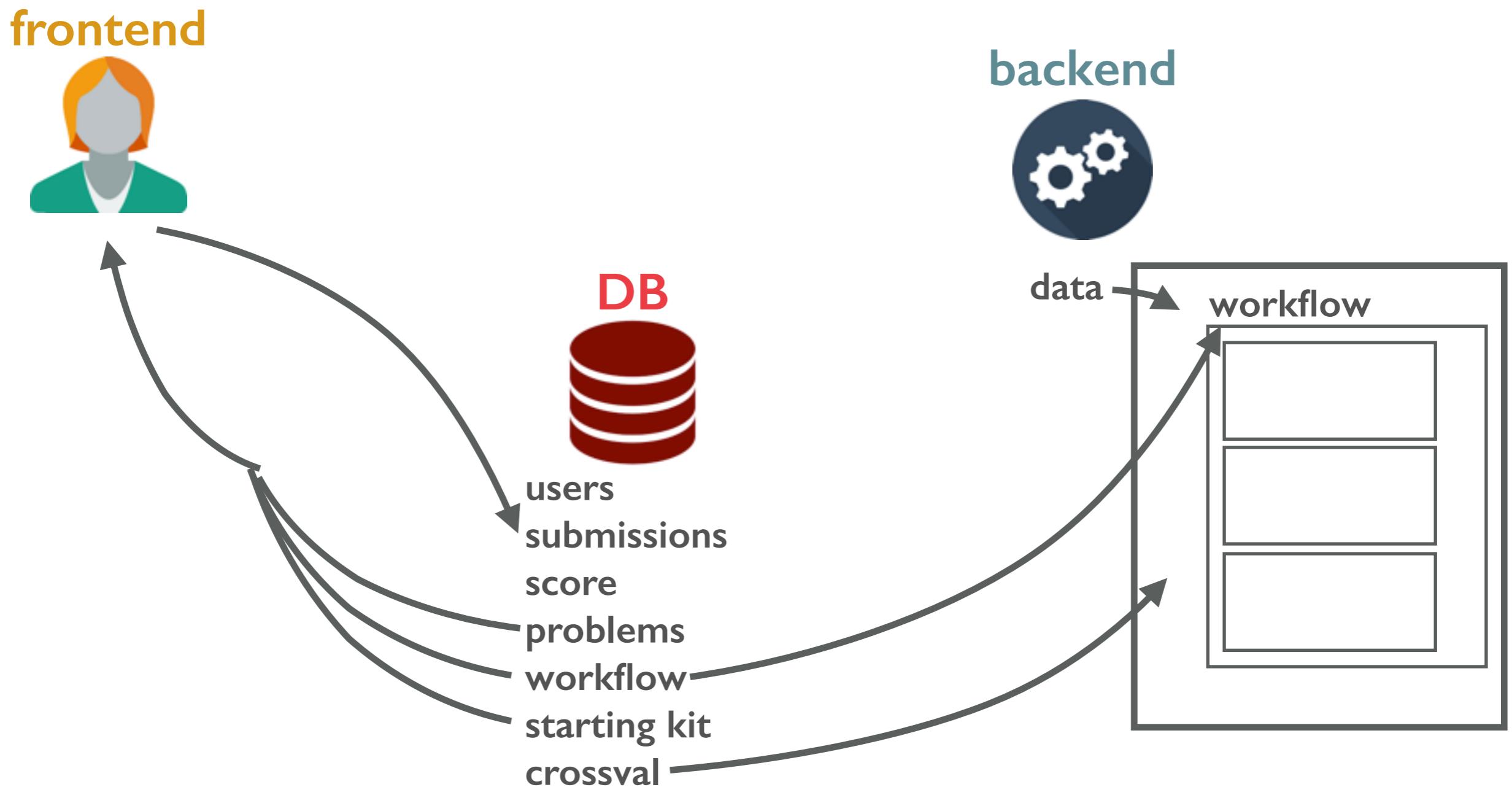
RAMP

DATA CHALLENGE WITH *CODE SUBMISSION*



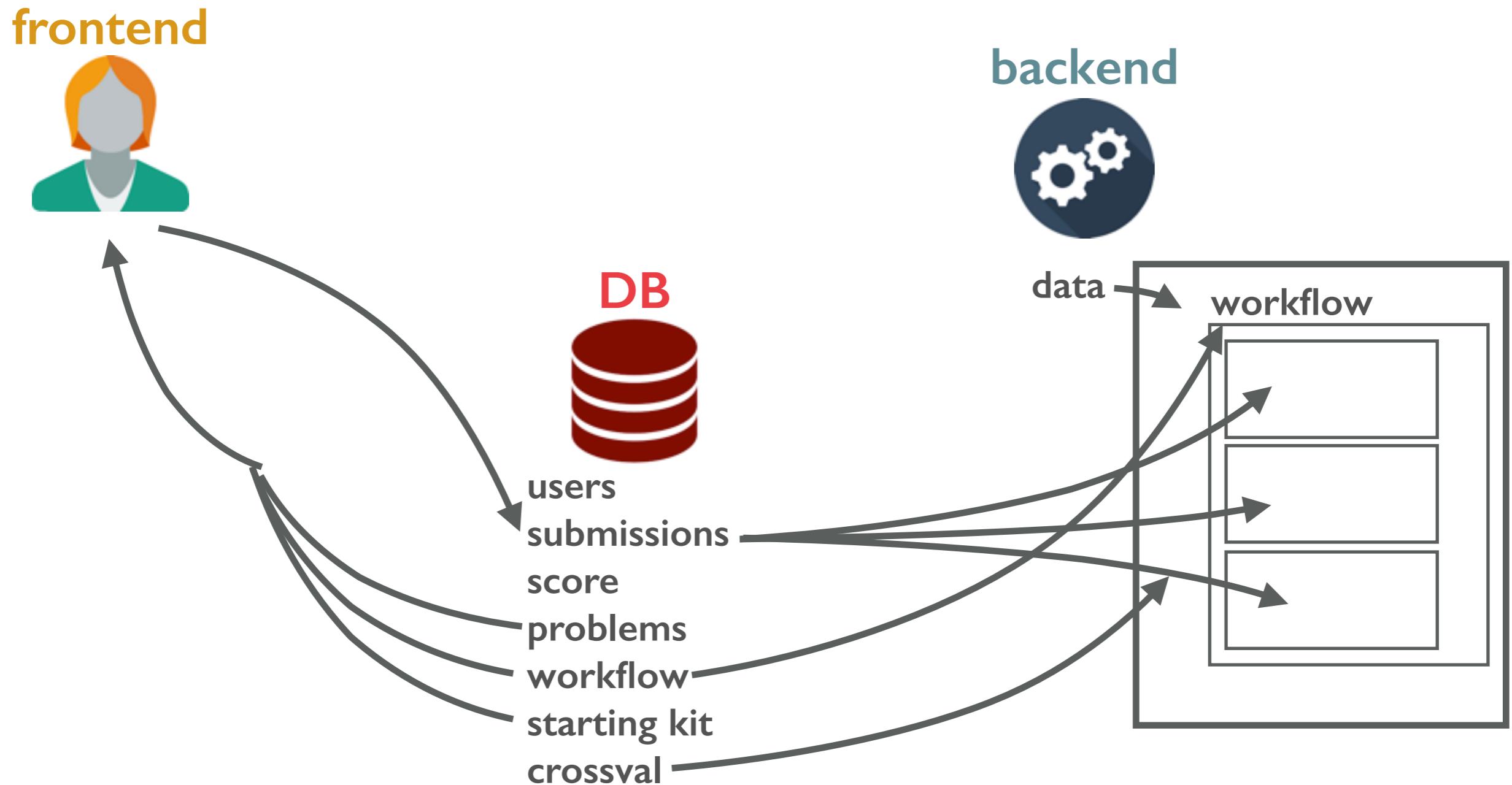
RAMP

DATA CHALLENGE WITH *CODE SUBMISSION*



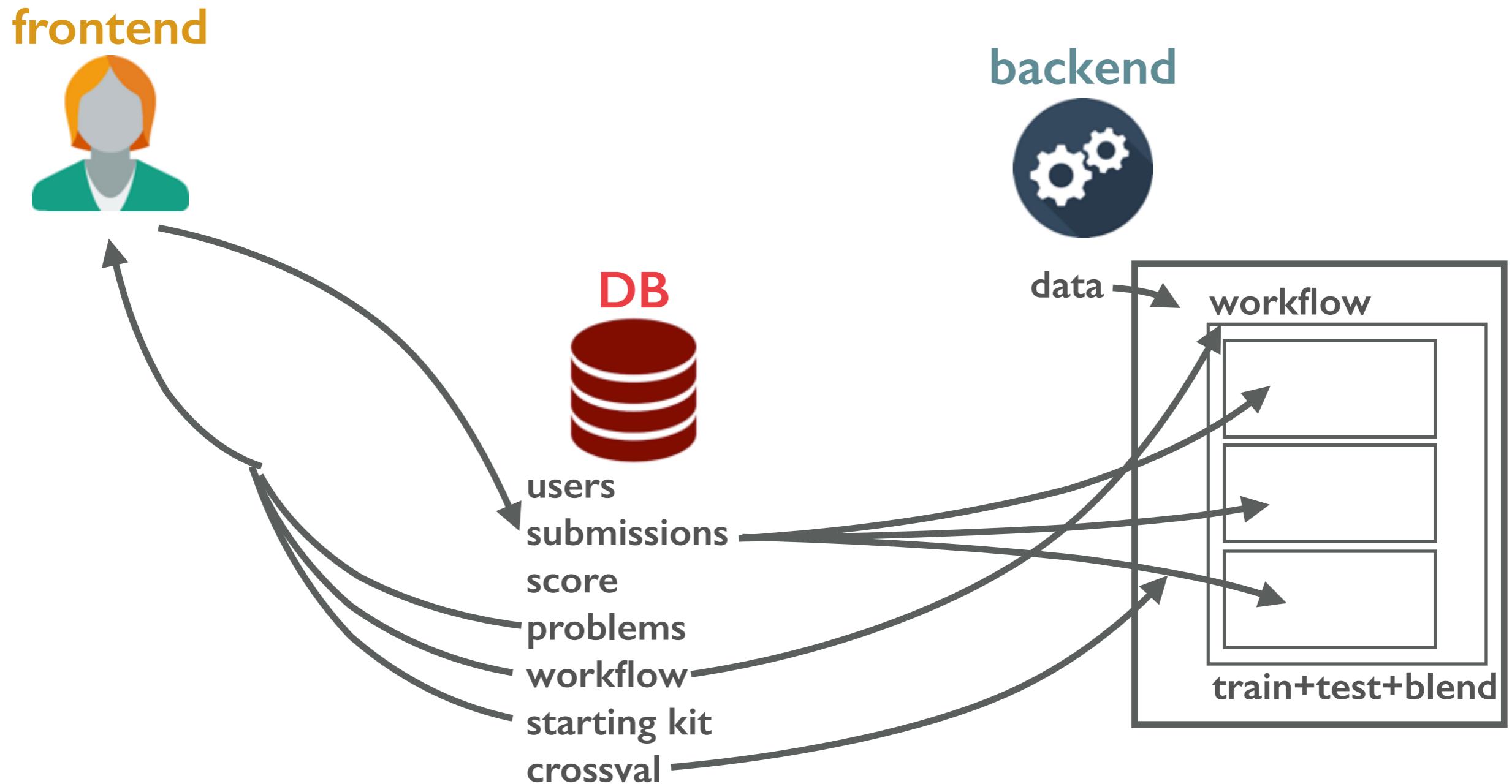
RAMP

DATA CHALLENGE WITH *CODE SUBMISSION*



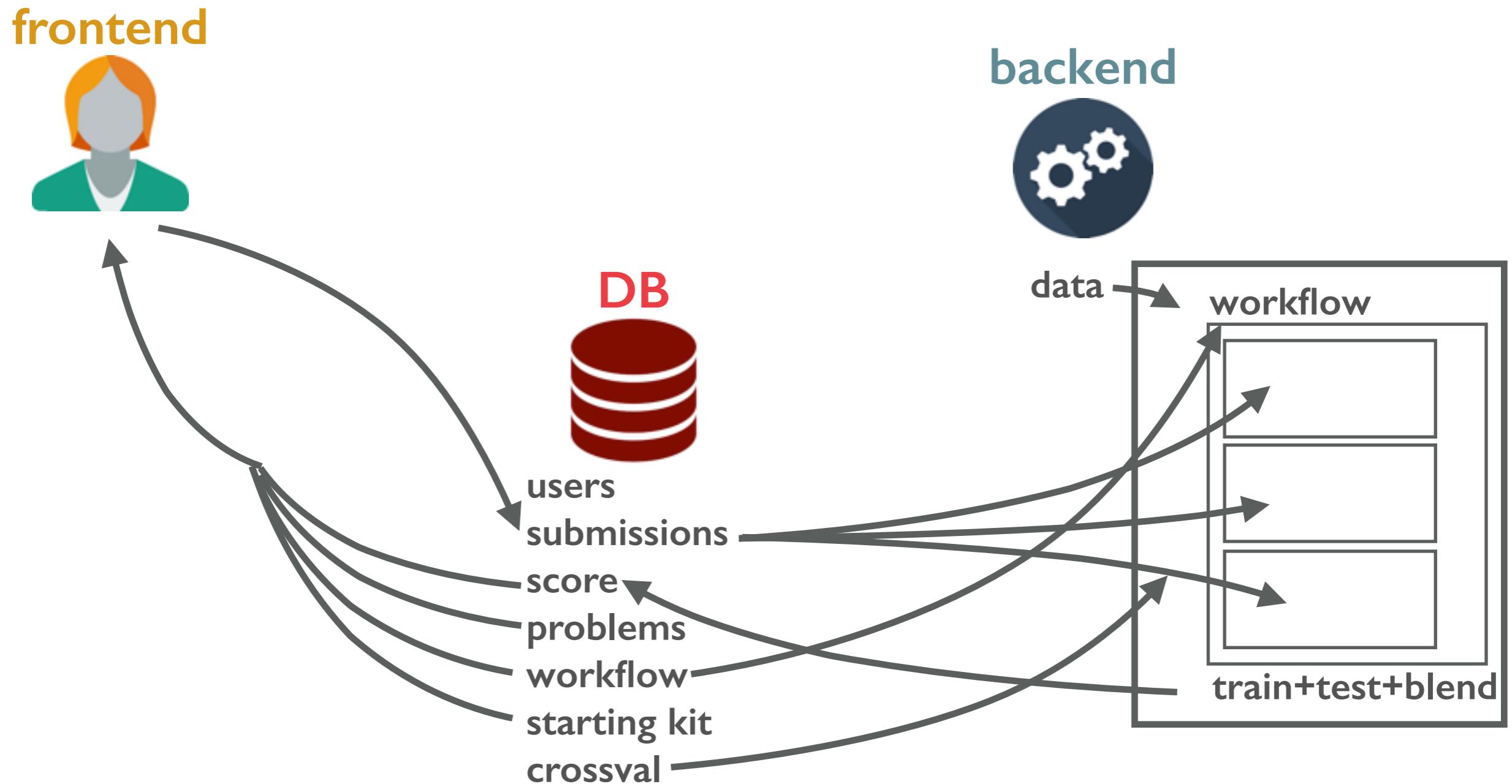
RAMP

DATA CHALLENGE WITH *CODE SUBMISSION*



RAMP

DATA CHALLENGE WITH *CODE SUBMISSION*





RAMP

Hi Balazs!



sea_ice_M1XMAP583_201617



Description



Balázs Kégl (CNRS), Camille Marini (CNRS), Andy Rhines (UW), Jennifer Dy (NEU), Arindam Banerjee (UMN)

Introduction

Arctic sea ice cover is one of the most variable features of Earth's climate. Its annual cycle peaks at around 15 million square kilometers in early spring, melting back to a minimum of about 6 million square kilometers in September. These seasonal swings are important for Earth's energy balance, as ice reflects the majority of sunlight while open water absorbs it. Changes in ice cover are also important for marine life and navigation for shipping.

Arctic Minimum (September 14, 2008)



Arctic Maximum (February 28, 2009)



Sea Ice Concentration (percent)



Sandbox

You can either edit and save the code in the left column or upload the files in the right column. You can also import code from other submissions when the leaderboard links are open.



Edit and save your code!



ts_feature_extractor

```
1 import numpy as np
2 import xarray as xr
3 from sklearn.linear_model import LinearRegression
4
5 class FeatureExtractor(object):
6
7     def __init__(self):
8         pass
9
10    def transform(self, X_ds):
11        """Compute the monthly averages of the ice_area, corresponding to the month
12        The code could be simplified but in this way it is general, can be used for
13        variables as well."""
14        # This is the range for which features should be provided. Strip
15        # the burn-in from the beginning and the prediction look-ahead from
16        # the end.
17        valid_range = np.arange(X_ds.attrs['n_burn_in'], len(X_ds['time']))
18
19        # We convert the Dataset into a 4D dataArray
20        X_xr = X_ds.to_array()
21
```

regressor

Upload your files!

File list

ts_feature_extractor.py

regressor.py

Upload file

No file chosen

① www.ramp.studio/events/sea_ice_M1XMAP583_201617/leaderboard

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RAMP

sea_ice_M1XMAP583_201617

Leaderboard

Combined score: 0.268

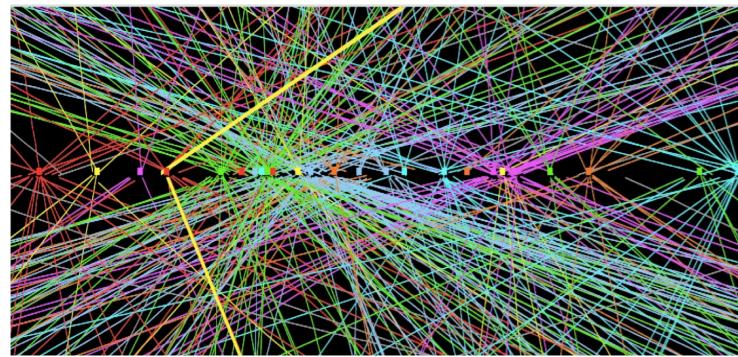
Show 10 entries Search:

team	submission	contributivity	historical contributivity	rmse	train time	test time	submitted at (UTC)
joseph.budin	noName	26	3	0.279	286	3	2017-02-13 11:36:28 Mon
alexis.thual	timeseries	16	16	0.296	1	1	2017-02-13 17:48:47 Mon
julien.habis	try_hard3	11	8	0.300	475	3	2017-02-13 19:45:35 Mon
kangzheng.liang	thirdtry	7	7	0.291	8	1	2017-02-07 19:11:32 Tue
joseph.budin	LinReg	6	3	0.280	234	3	2017-02-13 11:25:39 Mon
gaetan.millerand	shifted+boost+nino	6	5	0.295	29	5	2017-02-04 21:04:11 Sat
thibaut.vasseur	starting_kit_help	4	4	0.289	17	9	2017-02-13 18:48:37 Mon
yu-jia.cheong	Last	3	3	0.289	18	7	2017-02-13 13:28:53 Mon
gaetan.millerand	random_test	3	3	0.295	30	5	2017-02-07 13:12:29 Tue
maxime.lapides	TestFinal	3	3	0.296	458	3	2017-02-13 17:44:37 Mon

Showing 1 to 10 of 172 entries

Previous 1 2 3 4 5 ... 18 Next

ANOMALY DETECTION IN THE LHC ATLAS DETECTOR



reconstruction
+simulated anomalies

DER_mass_transverse_met_lep	1.937
DER_mass_vis	64.546
DER_pt_h	41.791
DER_deltar_tau_lep	2.301
DER_pt_tot	7.975
DER_sum_pt	105.305
DER_pt_ratio_lep_tau	0.926
DER_met_phi_centrality	1.087
PRI_tau_pt	36.259
PRI_tau_eta	-2.248
PRI_tau_phi	-2.239
PRI_lep_pt	33.582
PRI_lep_eta	-1.893
PRI_lep_phi	0.035
PRI_met	19.872
PRI_met_phi	-0.040
isSkewed	0.000



classifier

correct
(isSkewed = 0)

?

anomaly
(isSkewed = 1)

CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA



chemotherapy
drug in
elastic pocket

CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA



chemotherapy
drug in
elastic pocket



laser
spectrometer



CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA



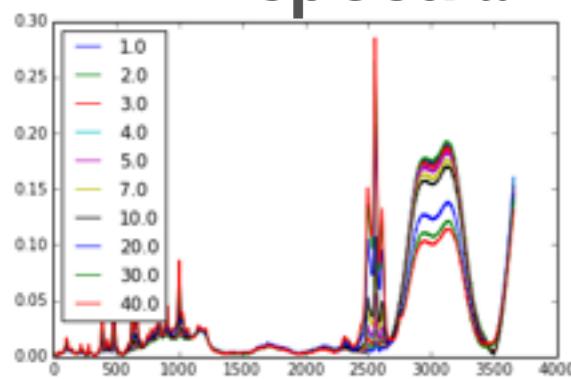
chemotherapy
drug in
elastic pocket



laser
spectrometer



molecular
spectra



CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA



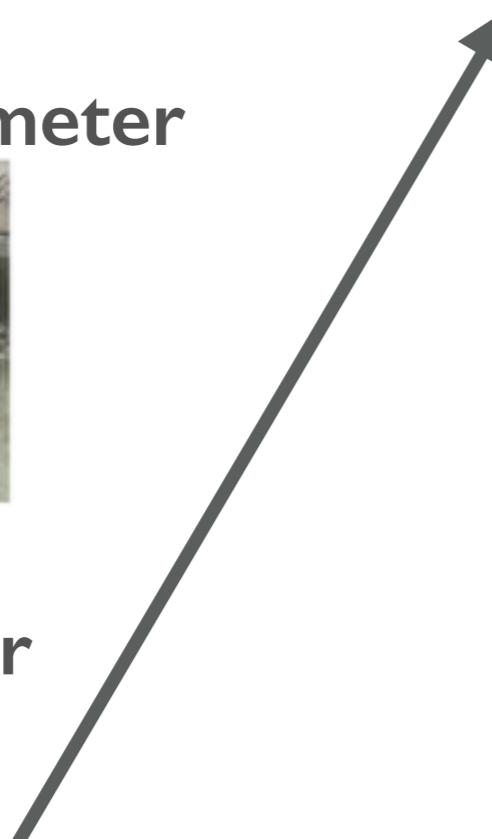
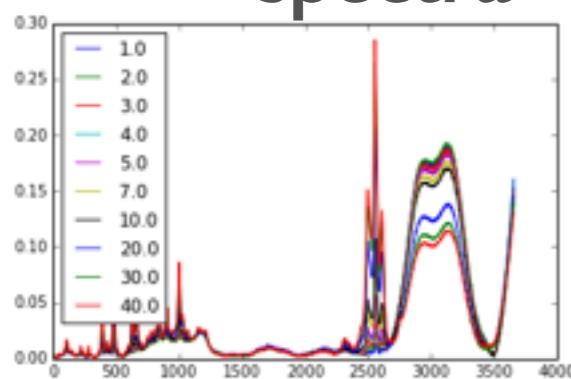
chemotherapy
drug in
elastic pocket

feature
extractor I

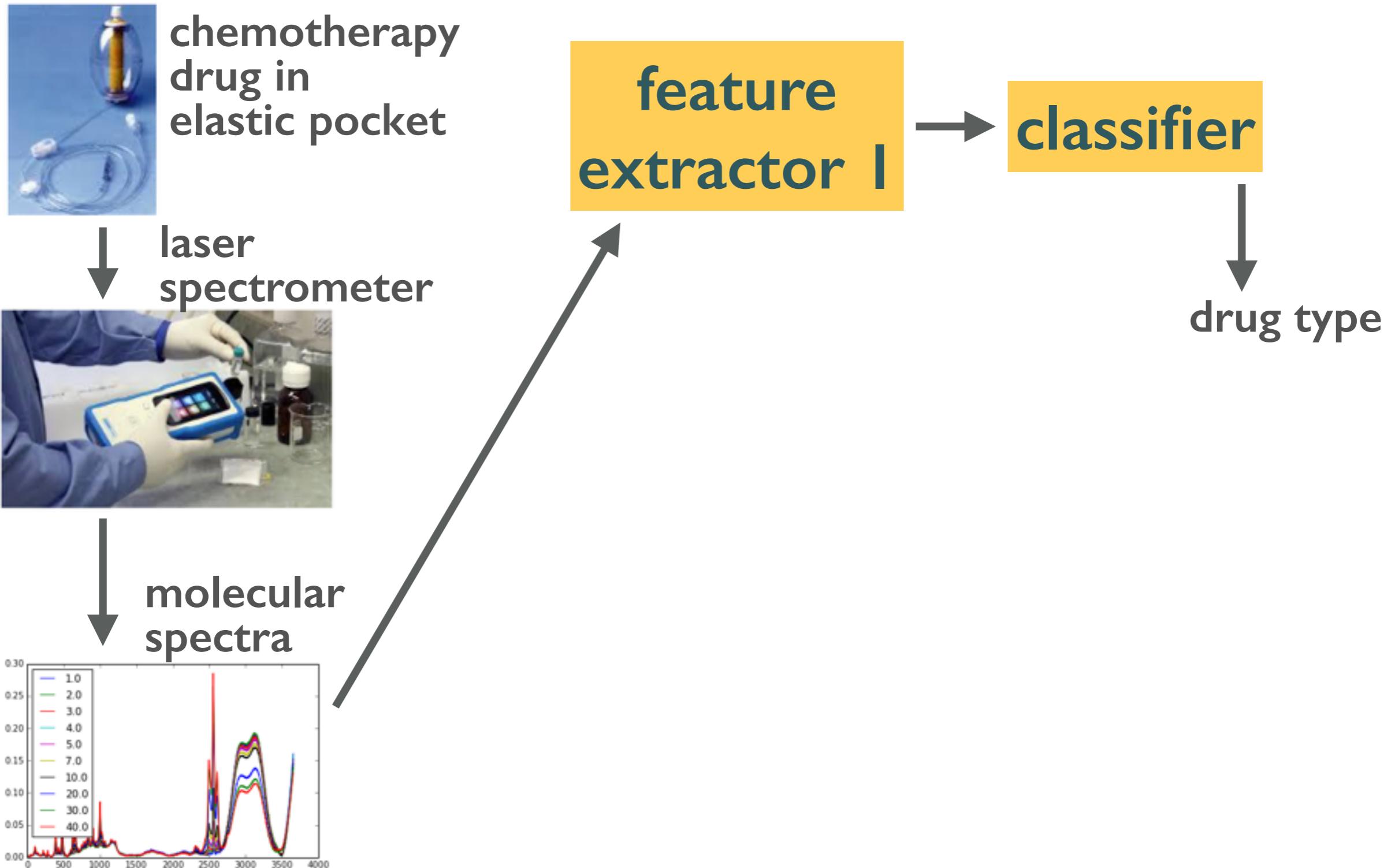
↓
laser
spectrometer



↓
molecular
spectra



CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA



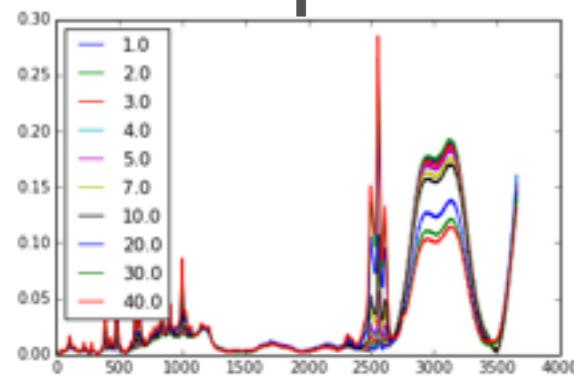
CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA



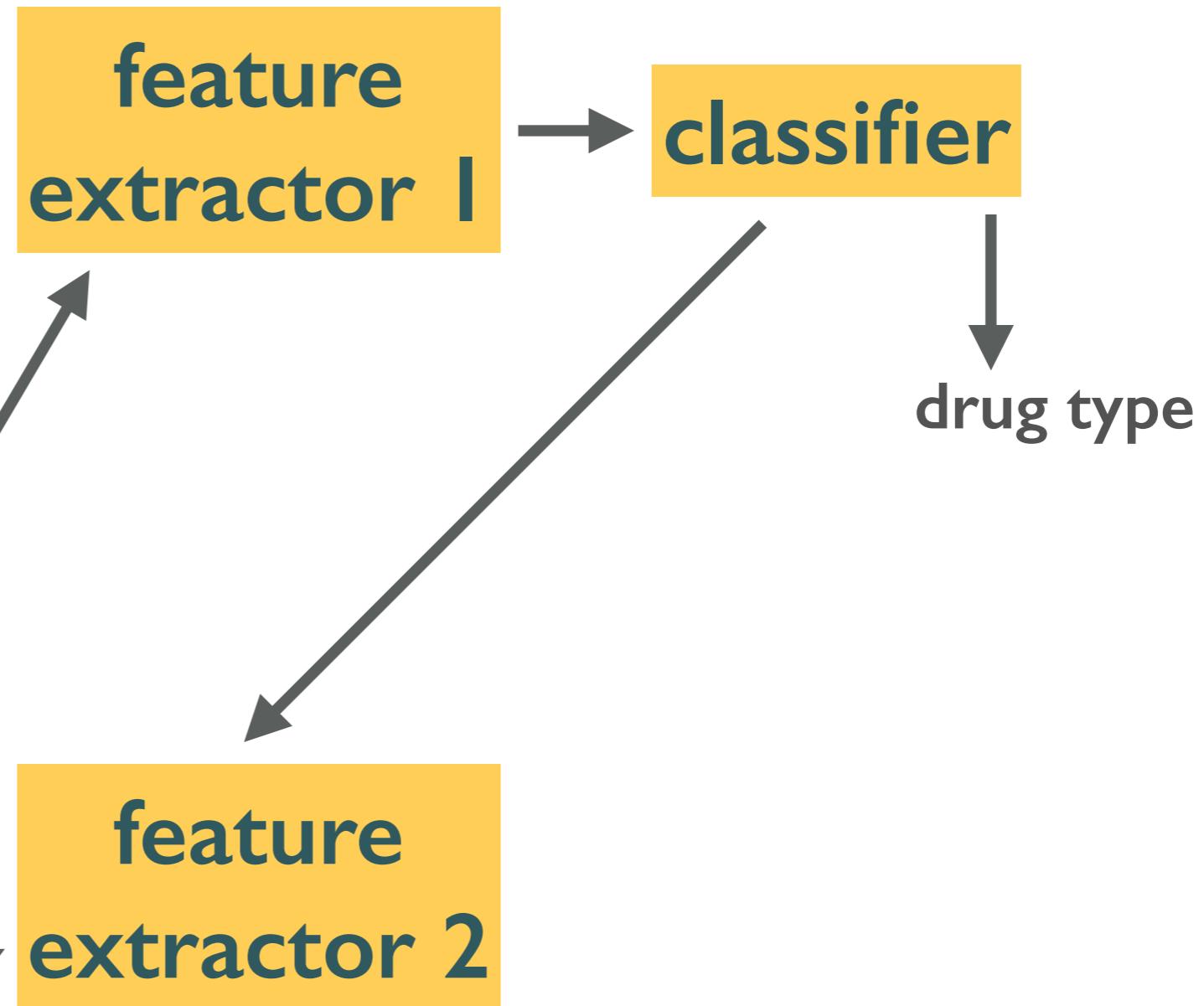
chemotherapy drug in elastic pocket



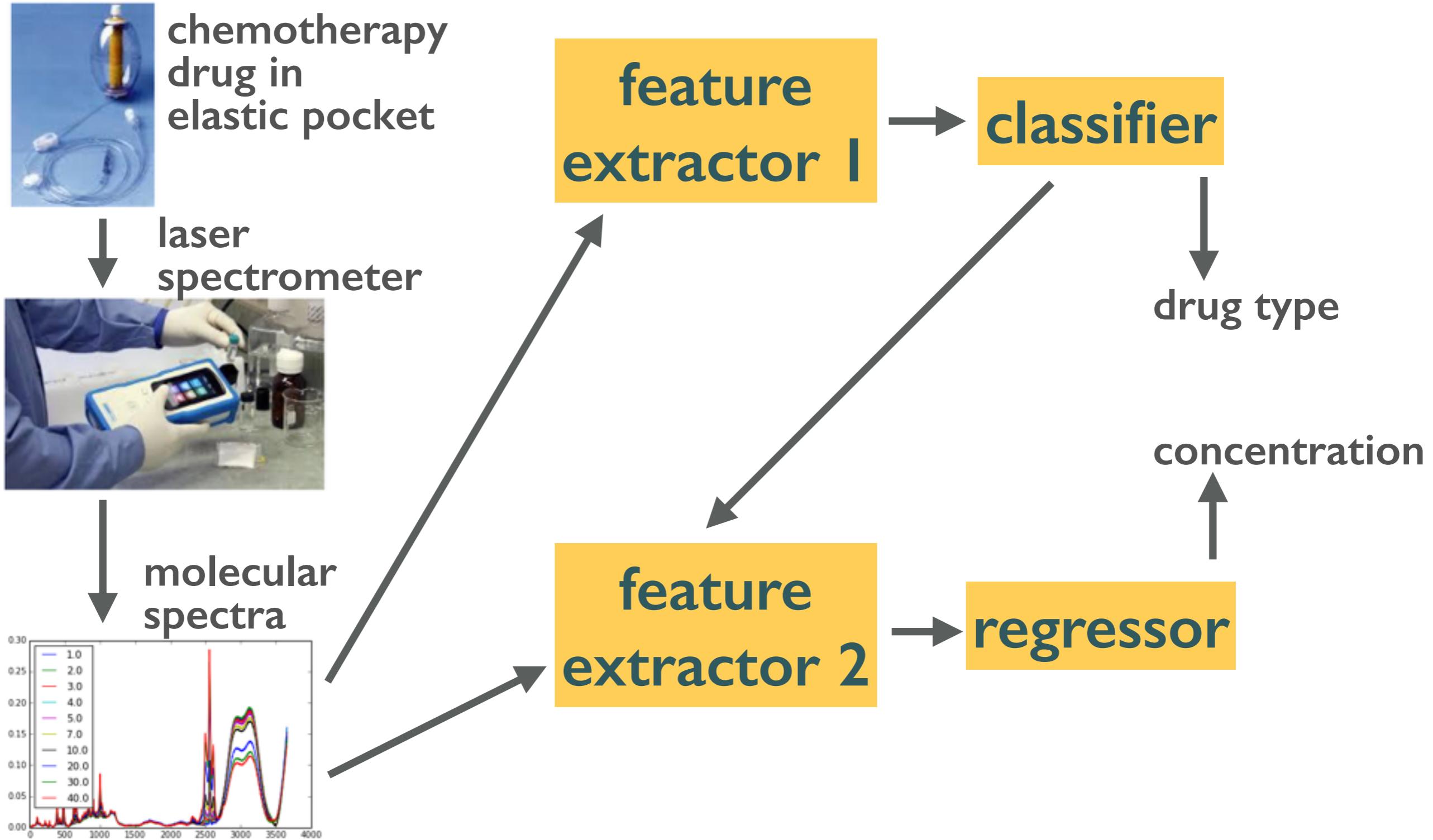
molecular spectra



laser spectrometer

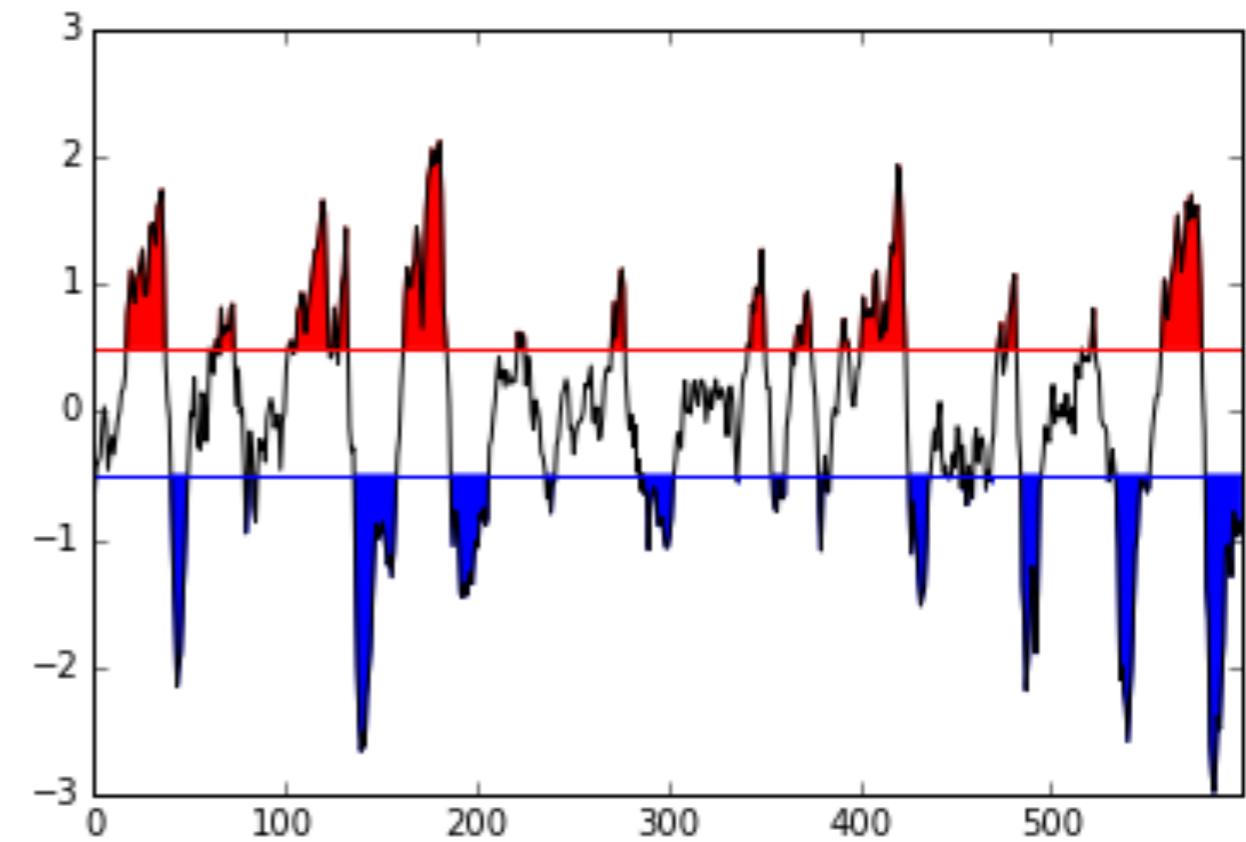
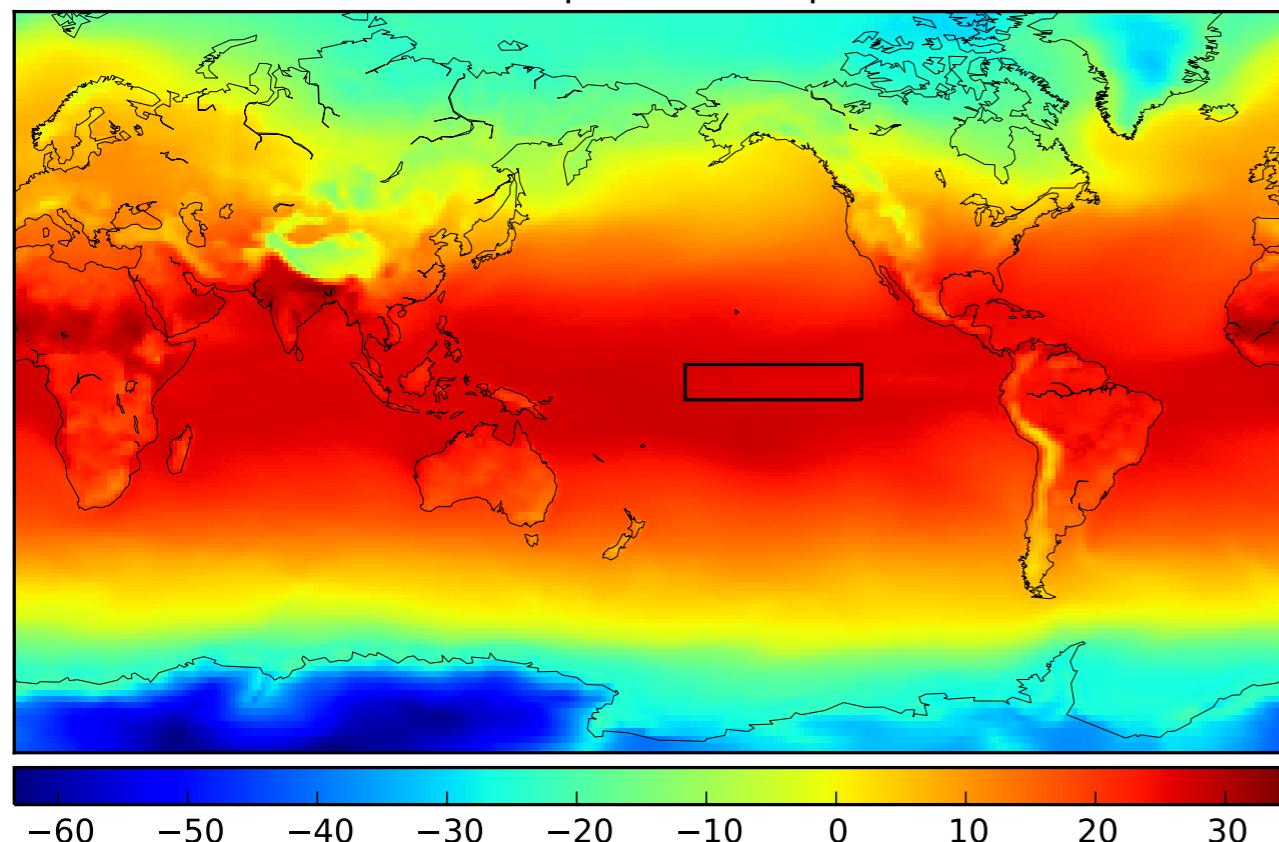


CLASSIFYING AND REGRESSING ON MOLECULAR SPECTRA



FORECASTING EL NIÑO SIX MONTHS AHEAD

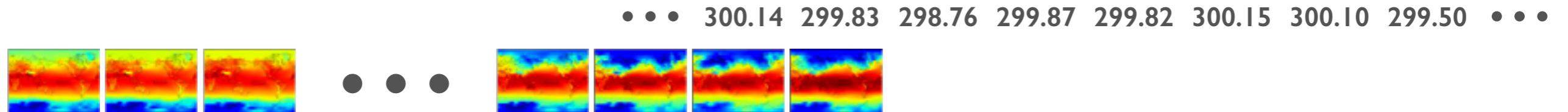
Temperature map



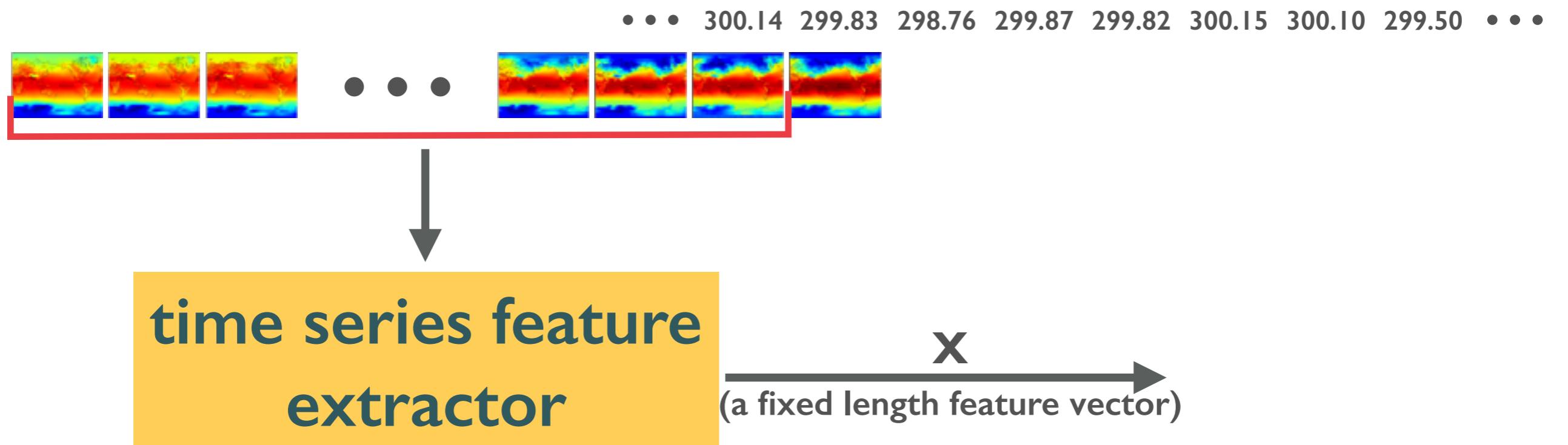
FORECASTING EL NIÑO SIX MONTHS AHEAD



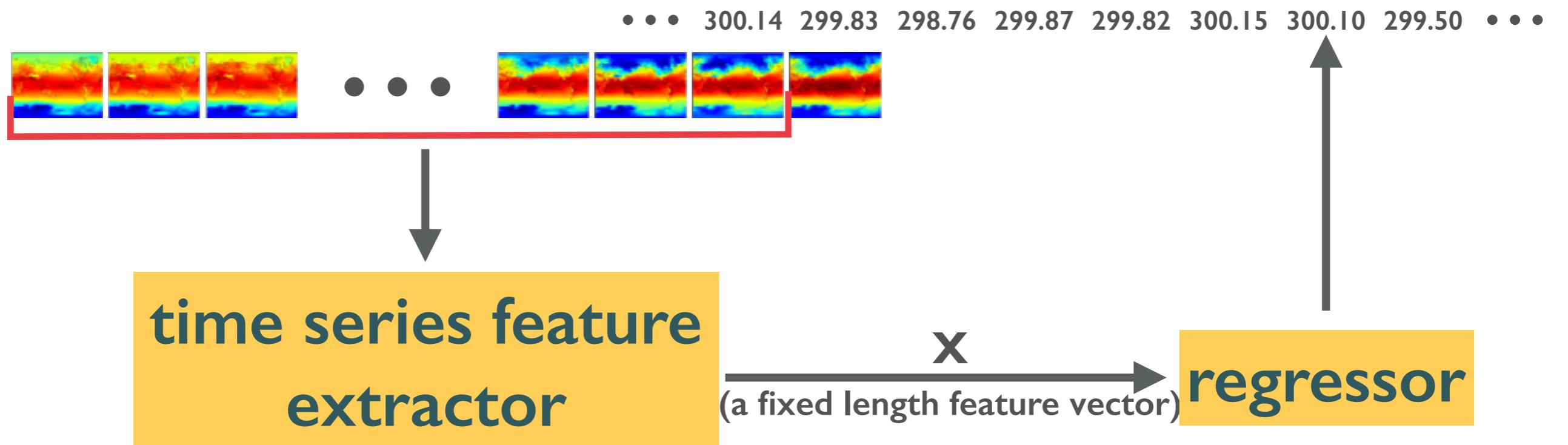
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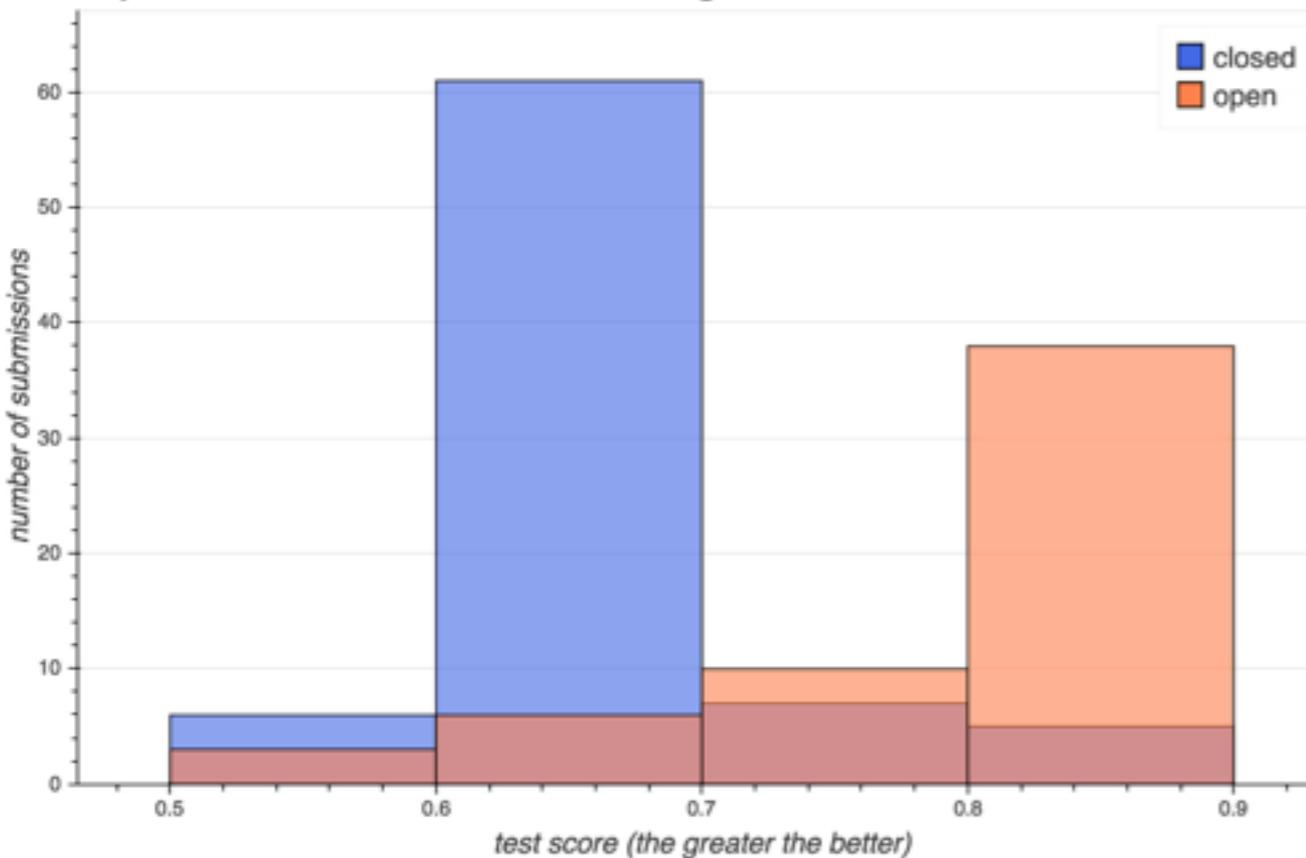
FORECASTING EL NIÑO SIX MONTHS AHEAD



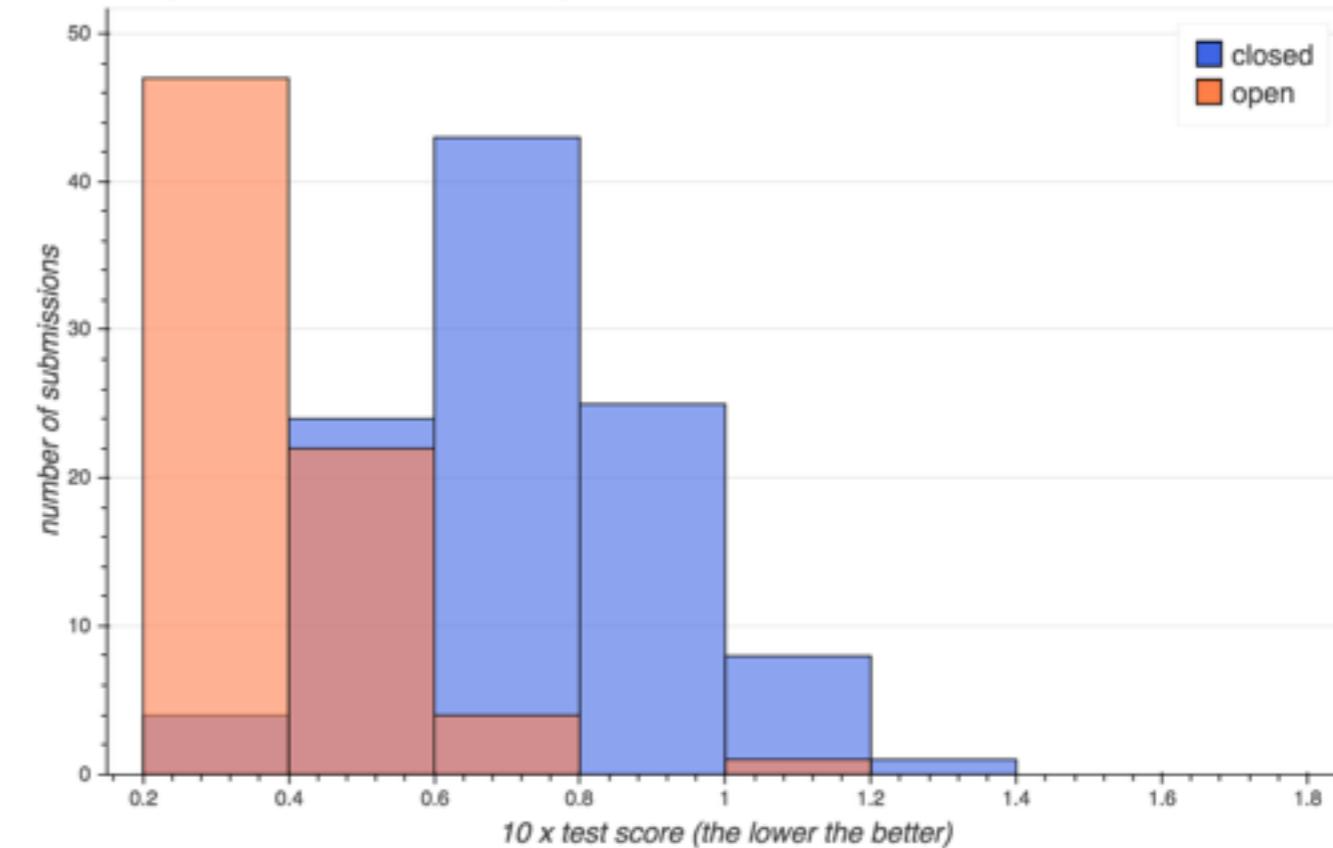
Analyzing the process

OPEN PHASE LETS PARTICIPANTS CATCH UP

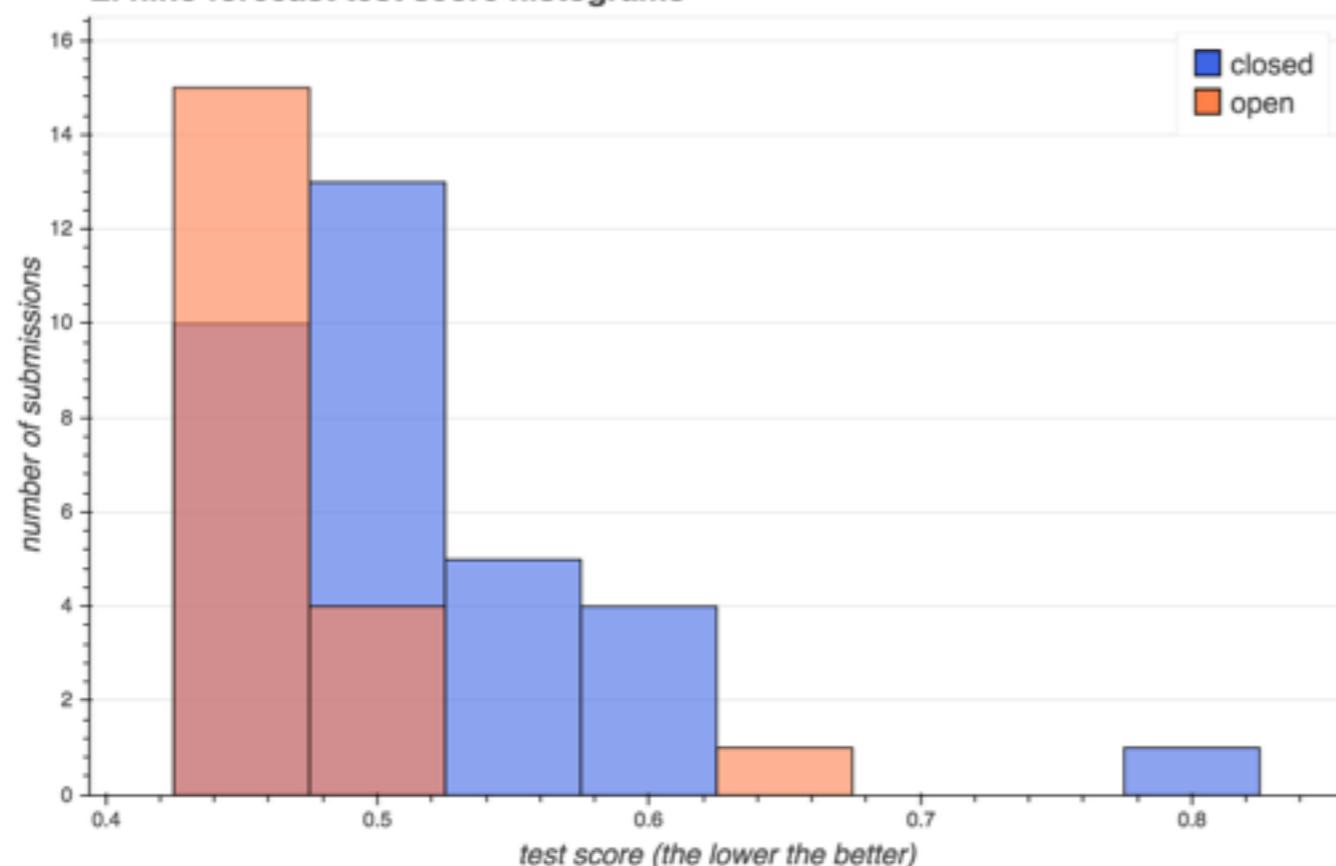
Hep detector anomalies test score histograms



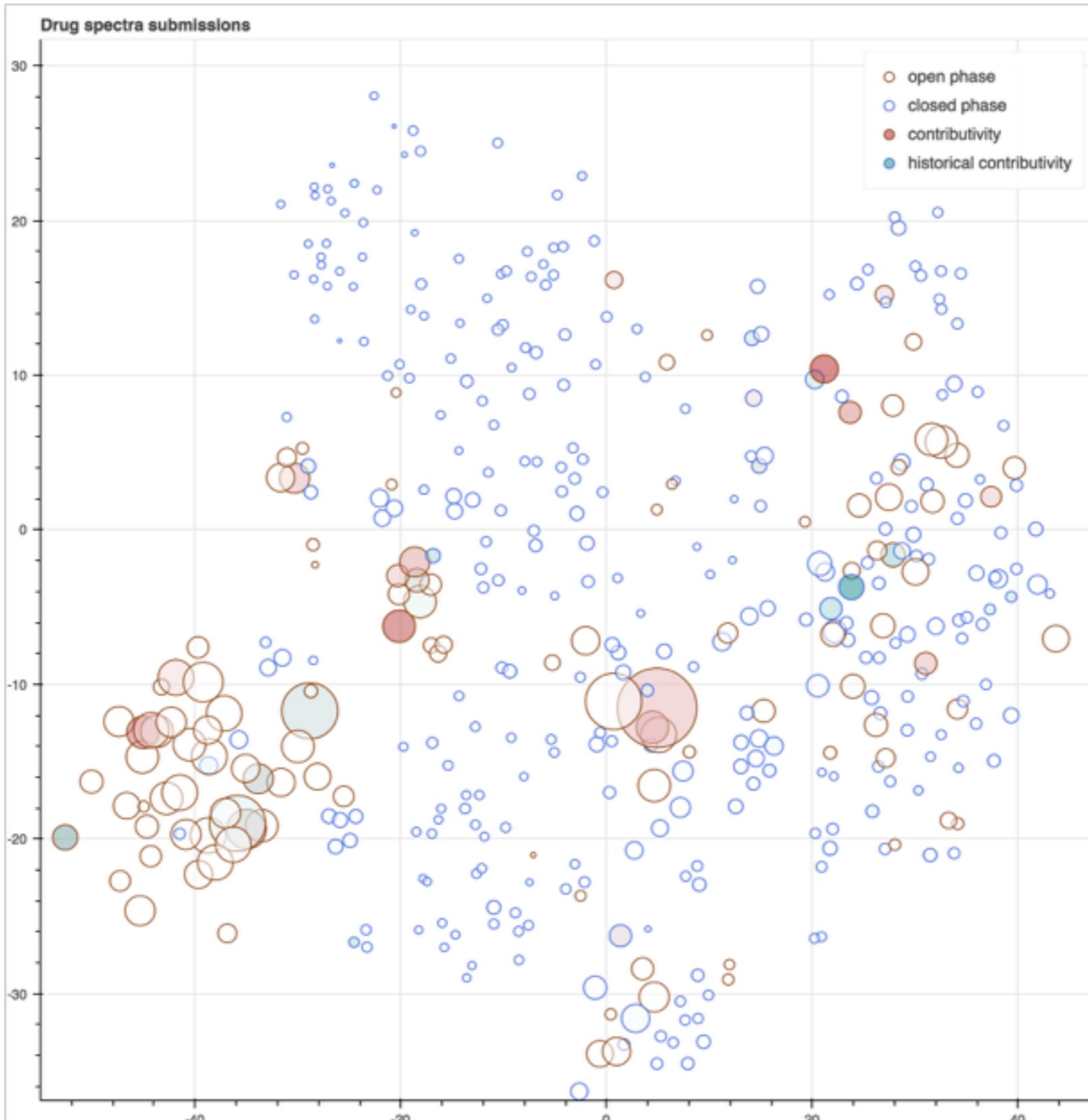
Drug spectra test score histograms



El nino forecast test score histograms



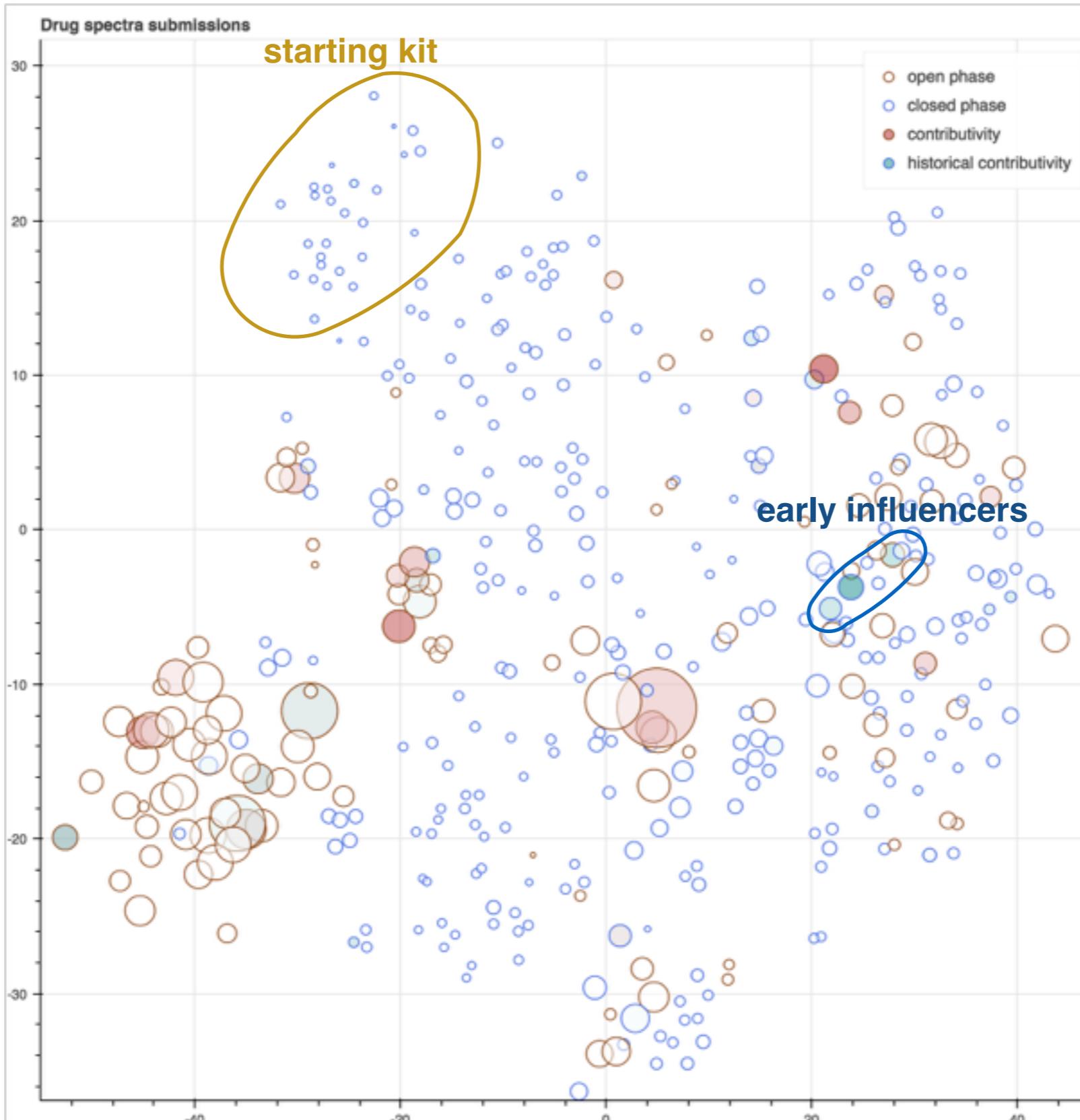
THE DYNAMICS OF COLLABORATION



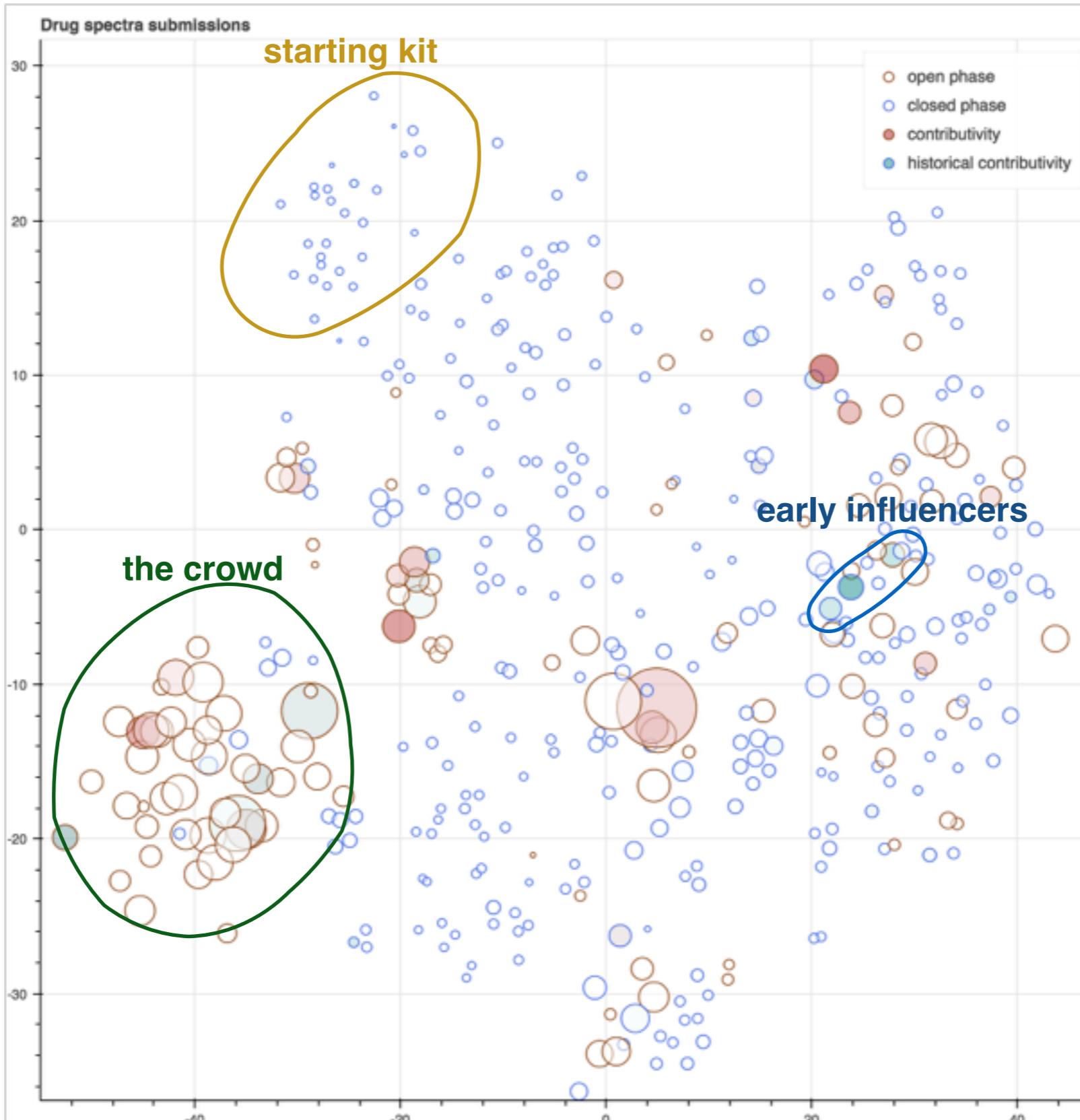
THE DYNAMICS OF COLLABORATION



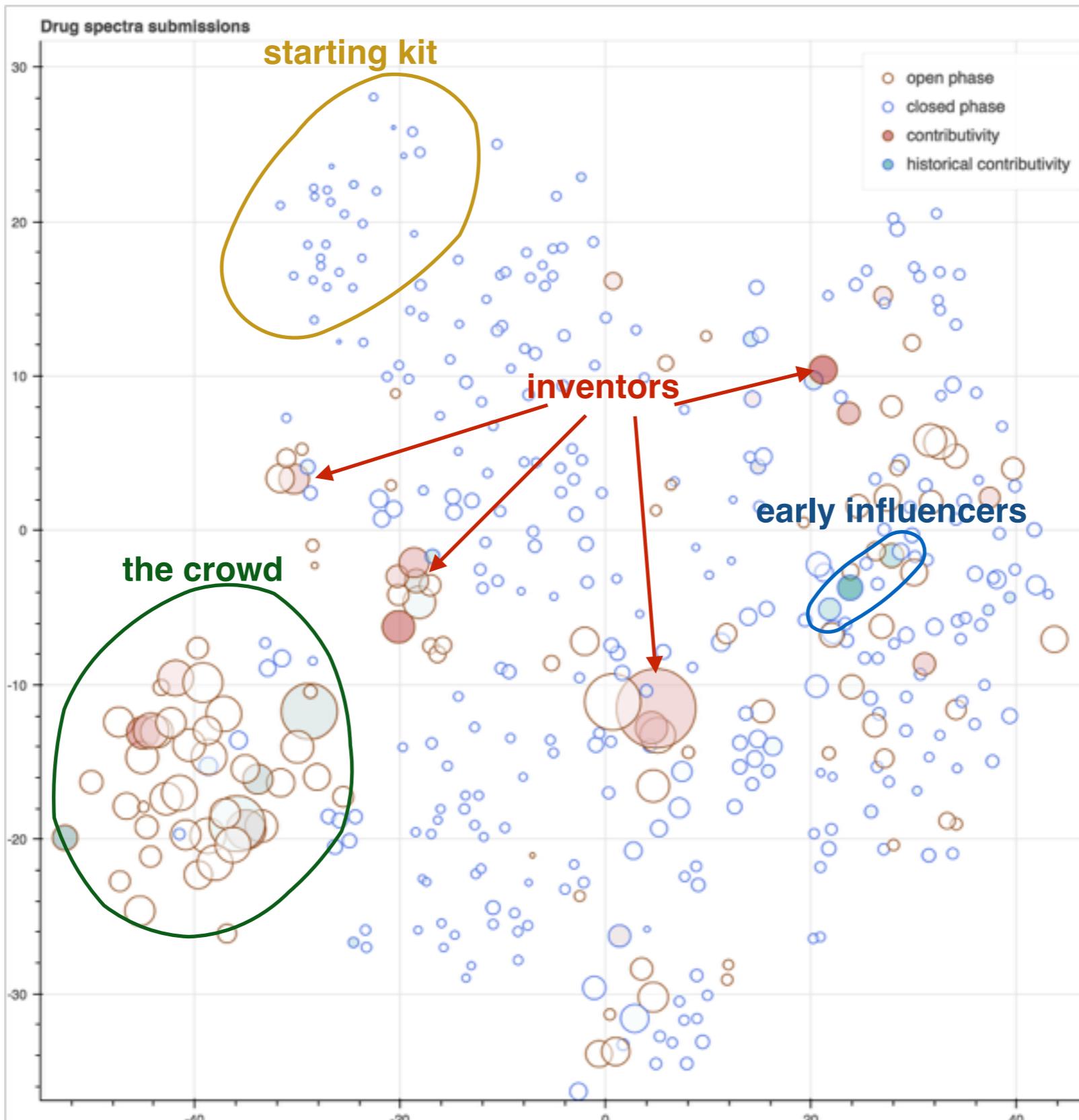
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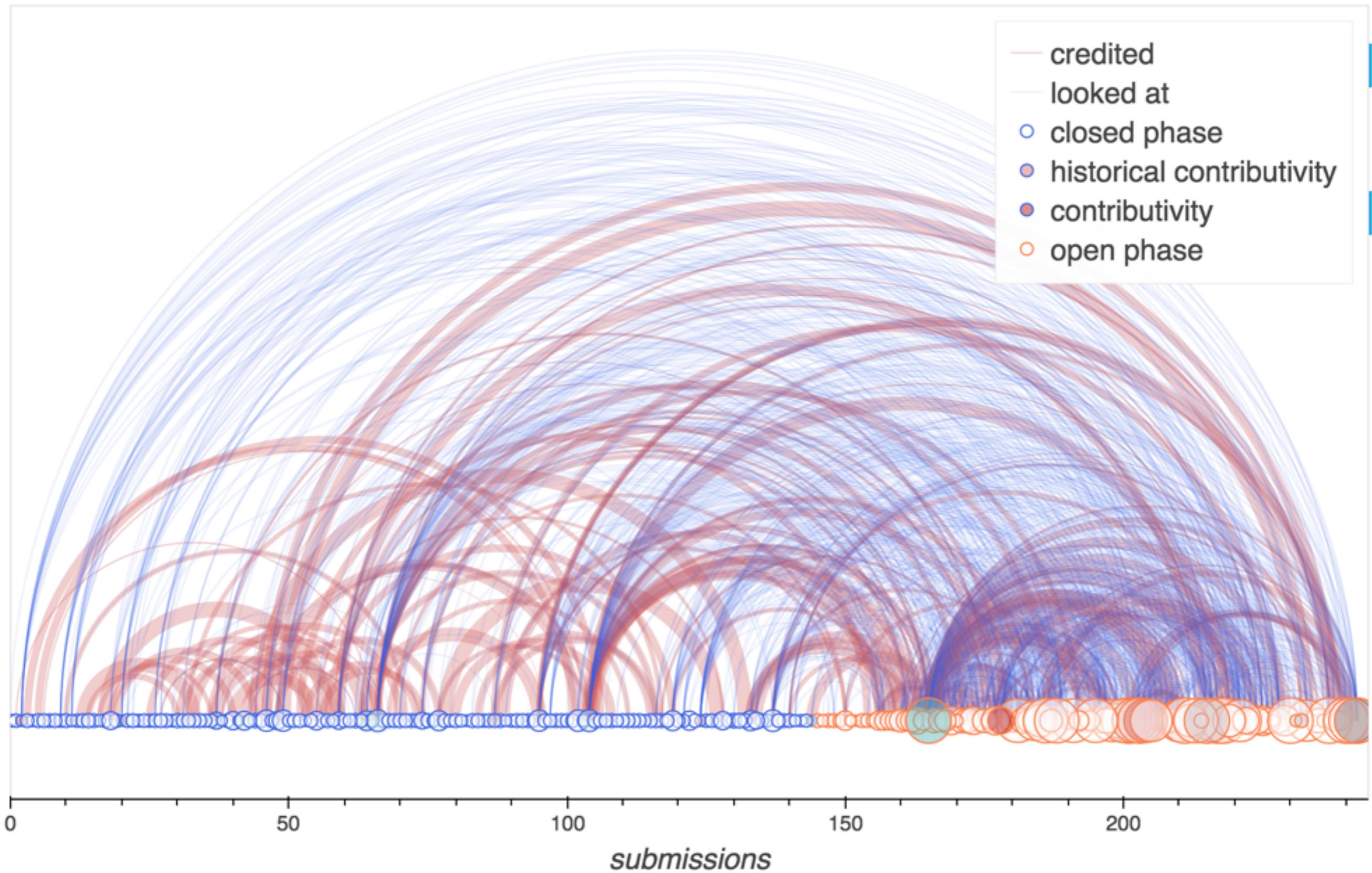


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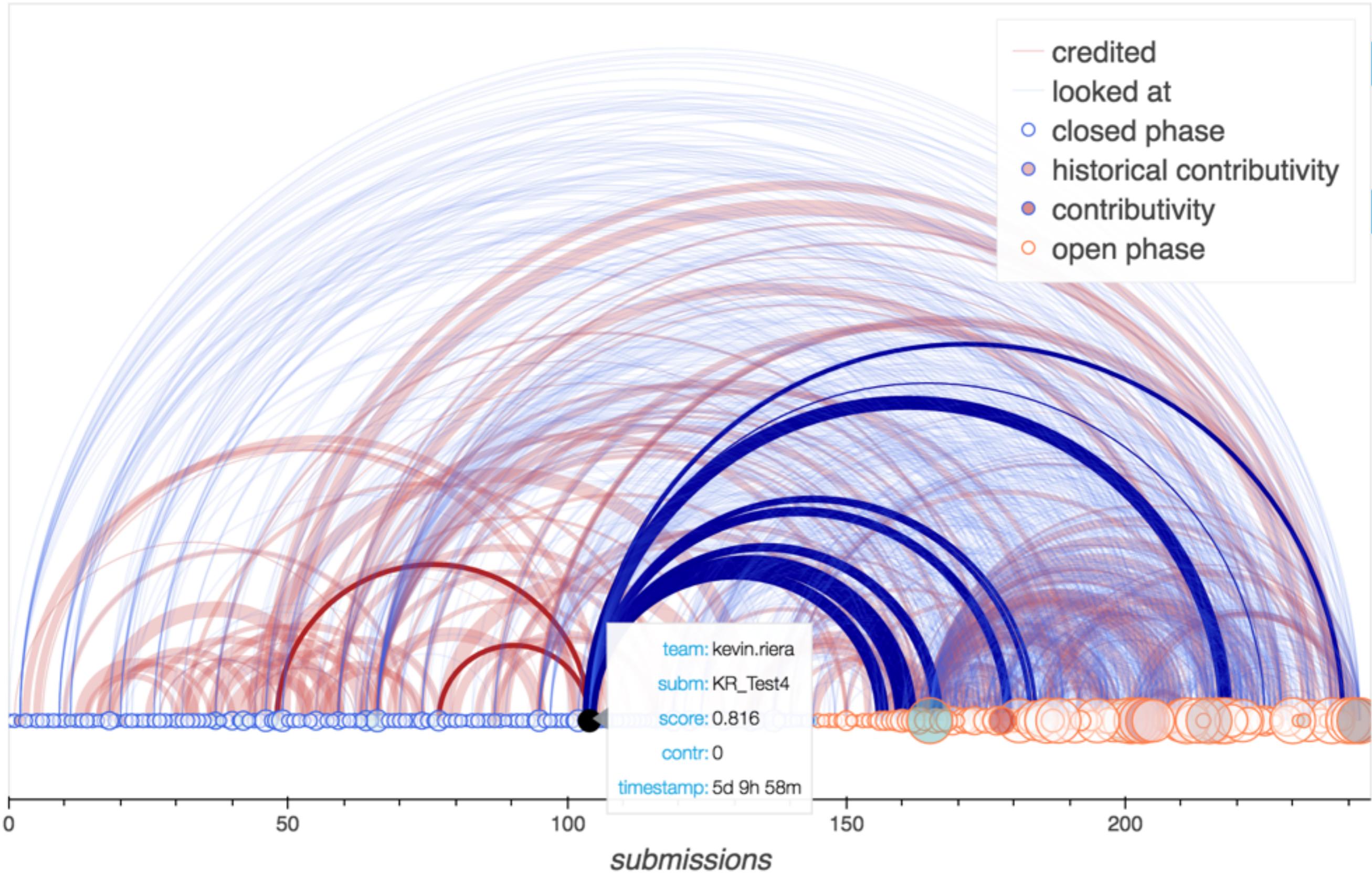
THE DYNAMICS OF COLLABORATION

Hep detector anomalies submissions



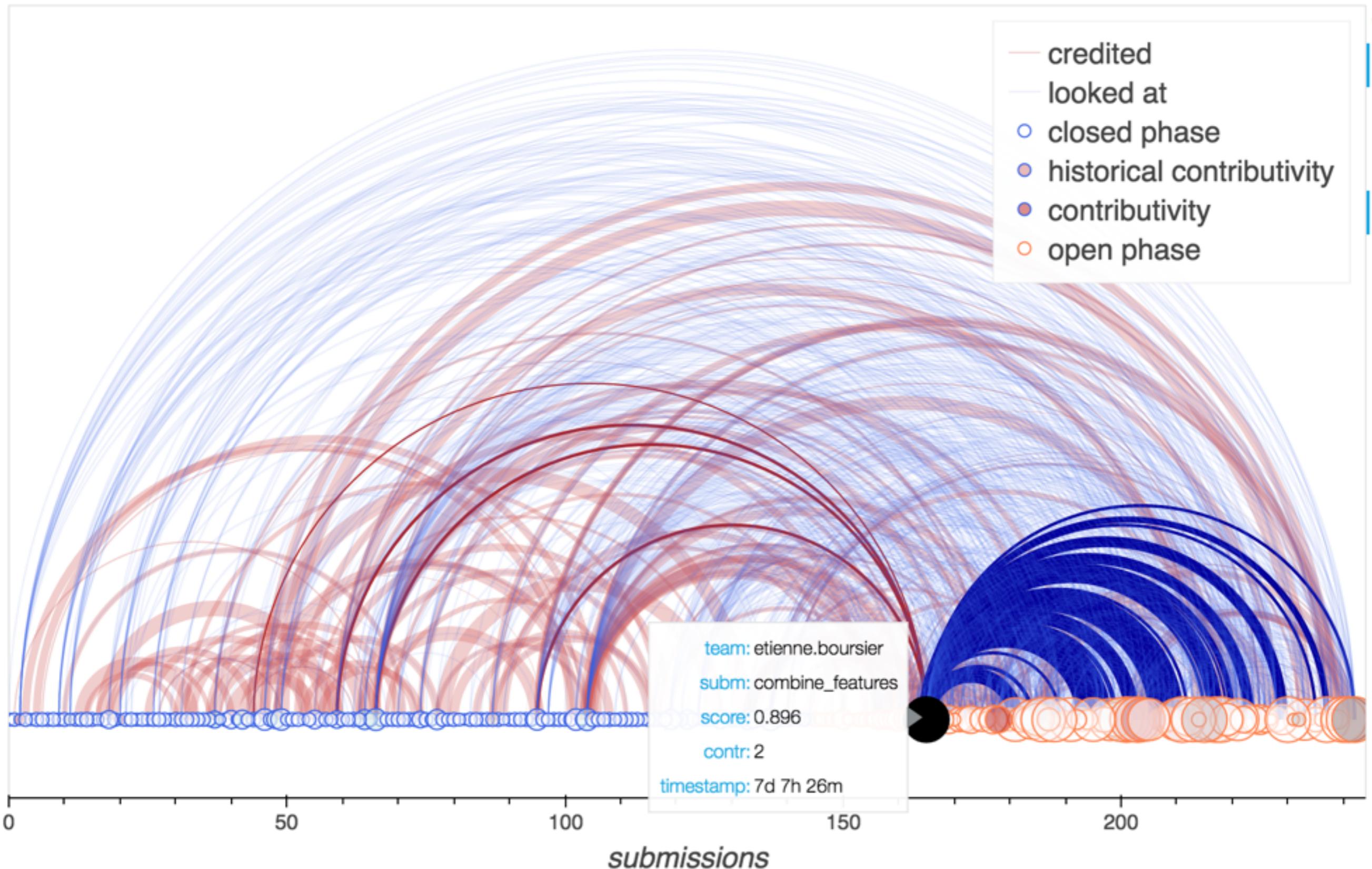
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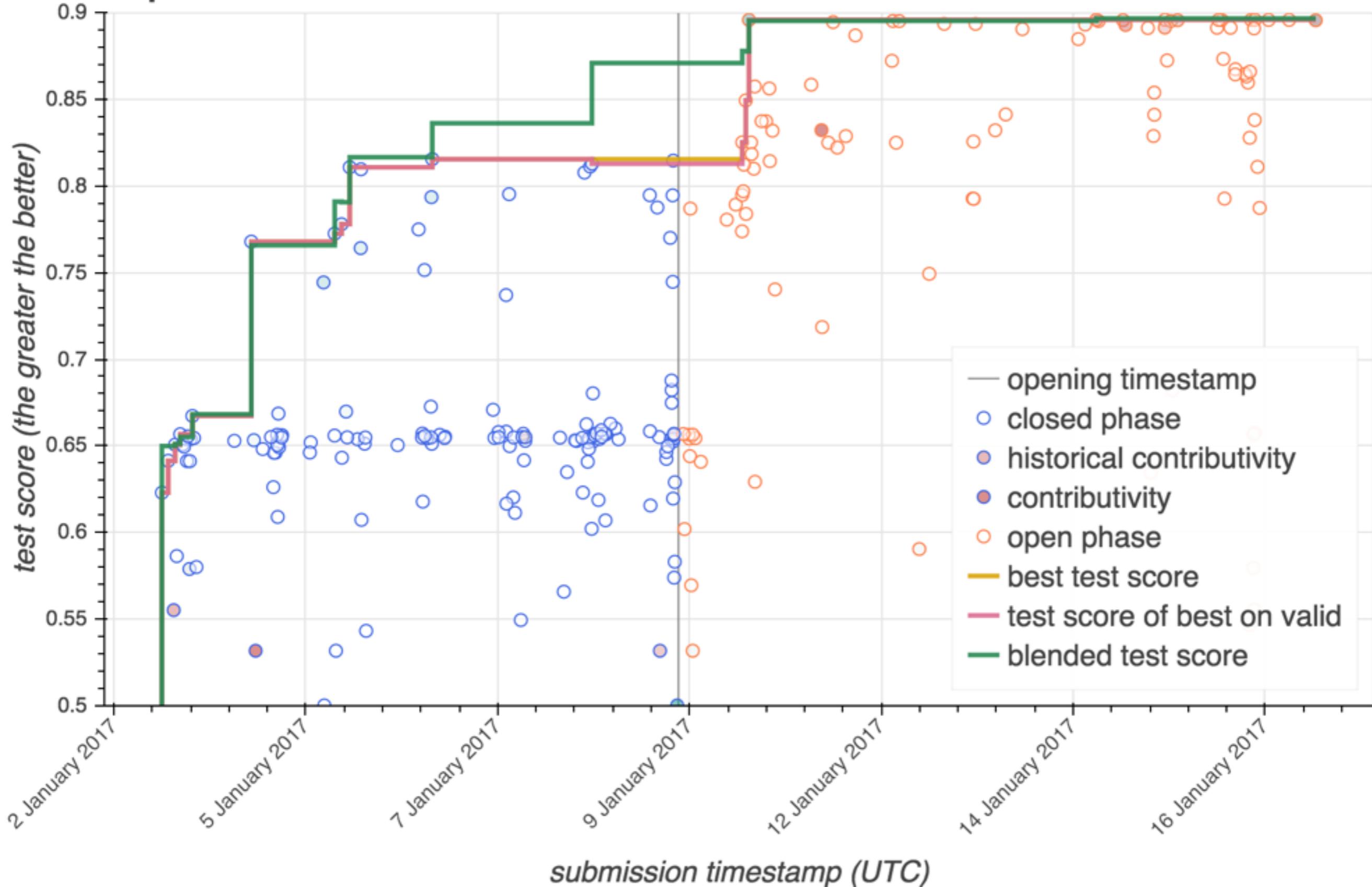


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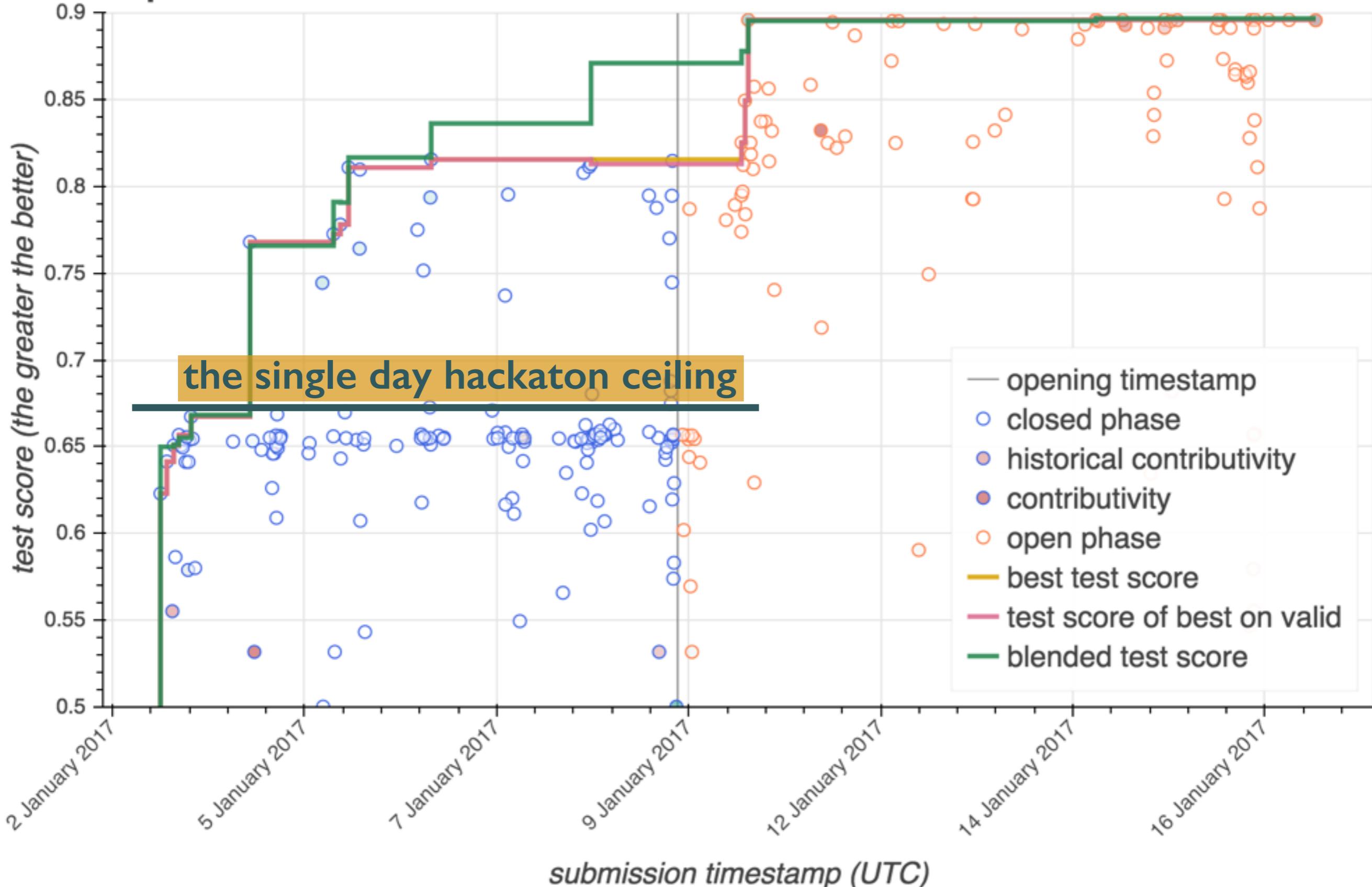
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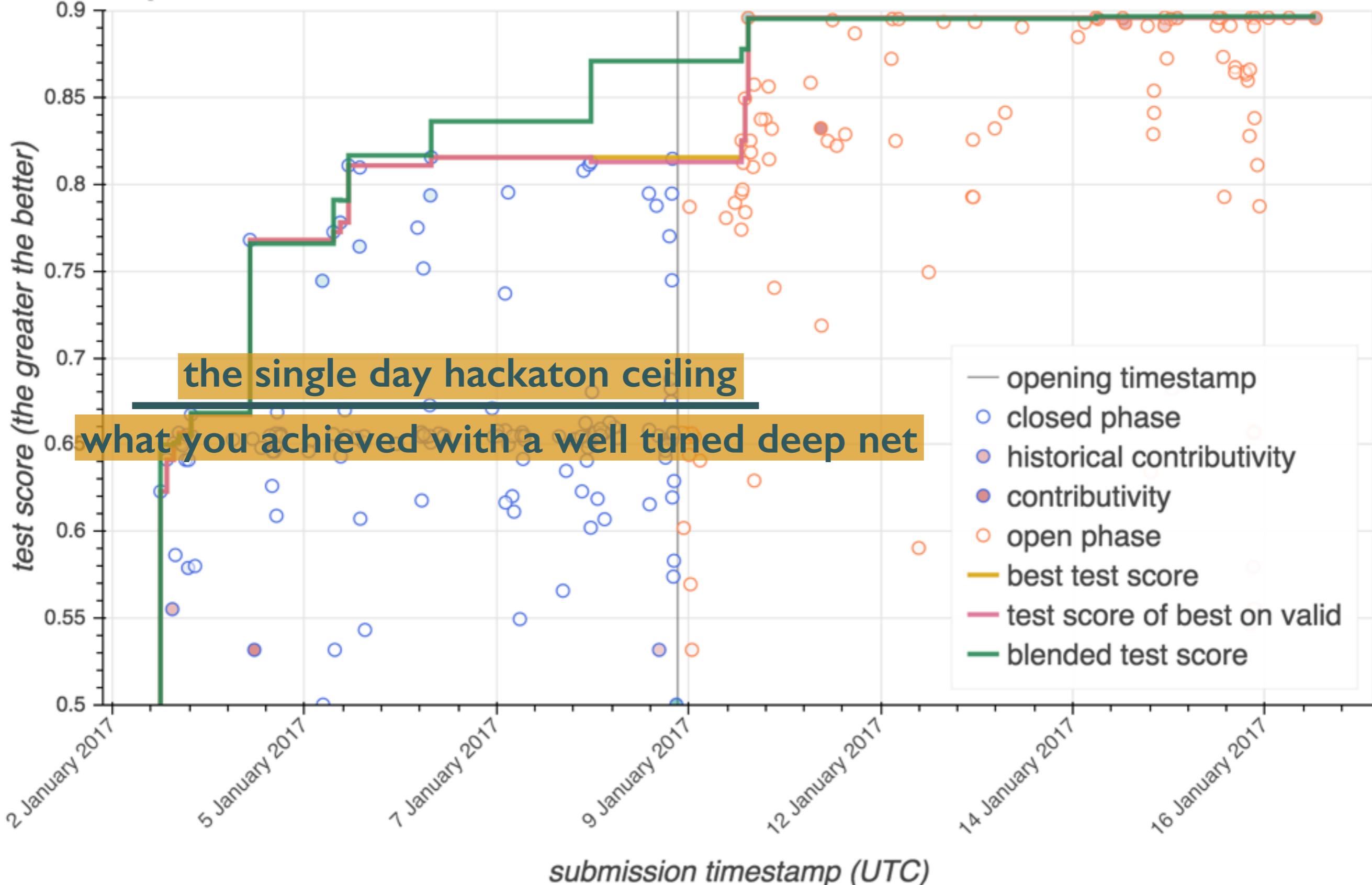
Hep detector anomalies test scores



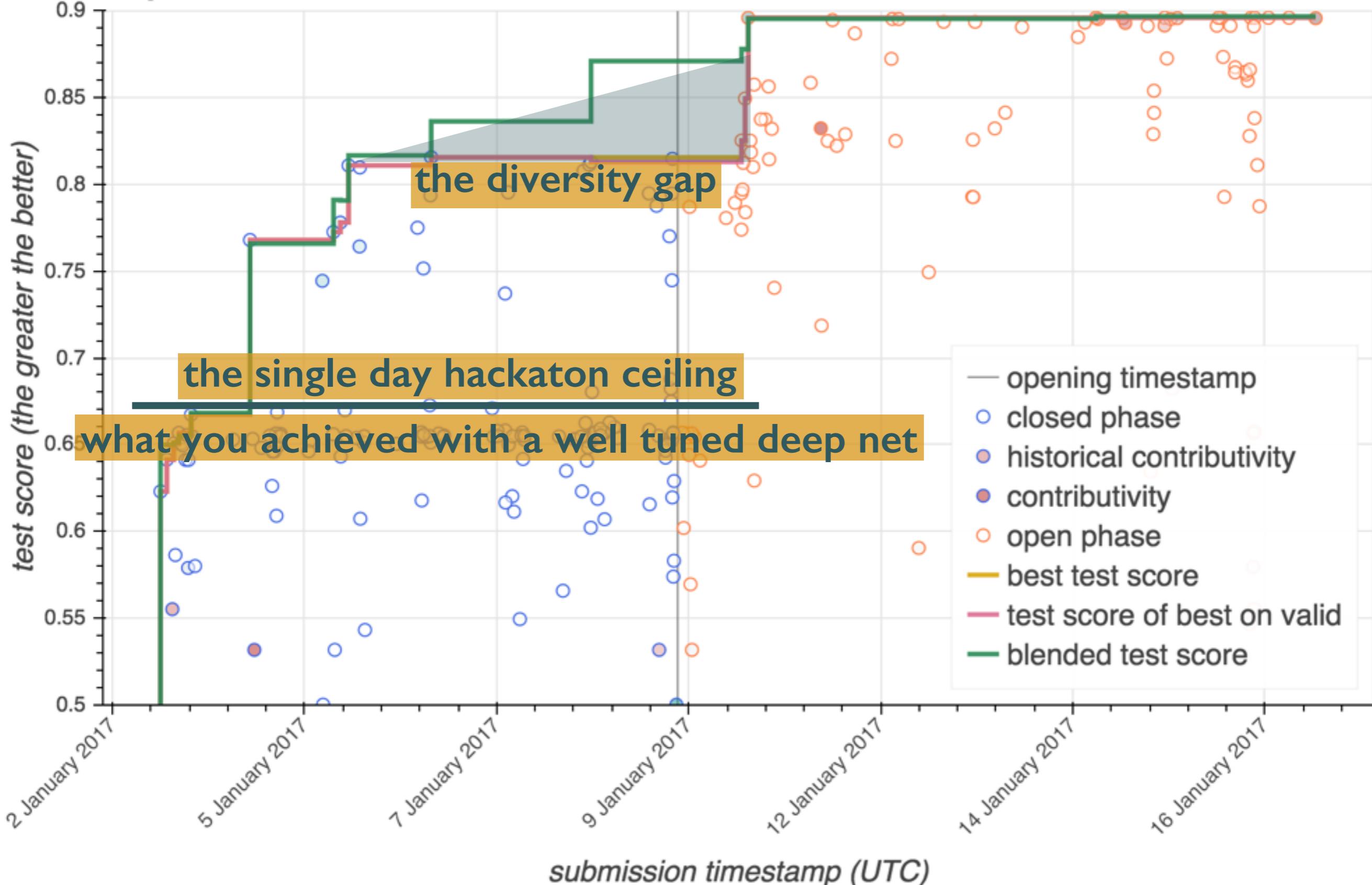
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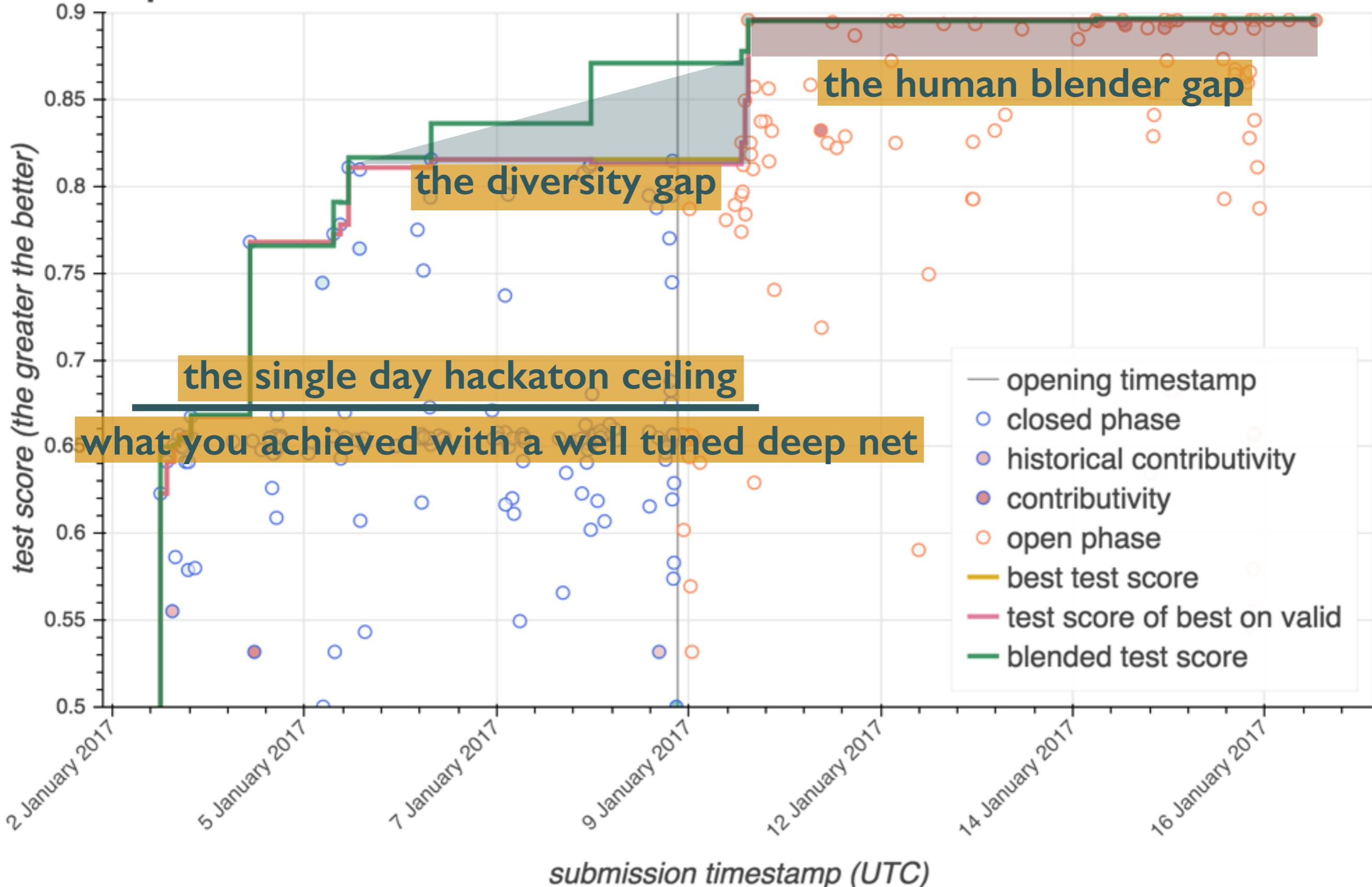
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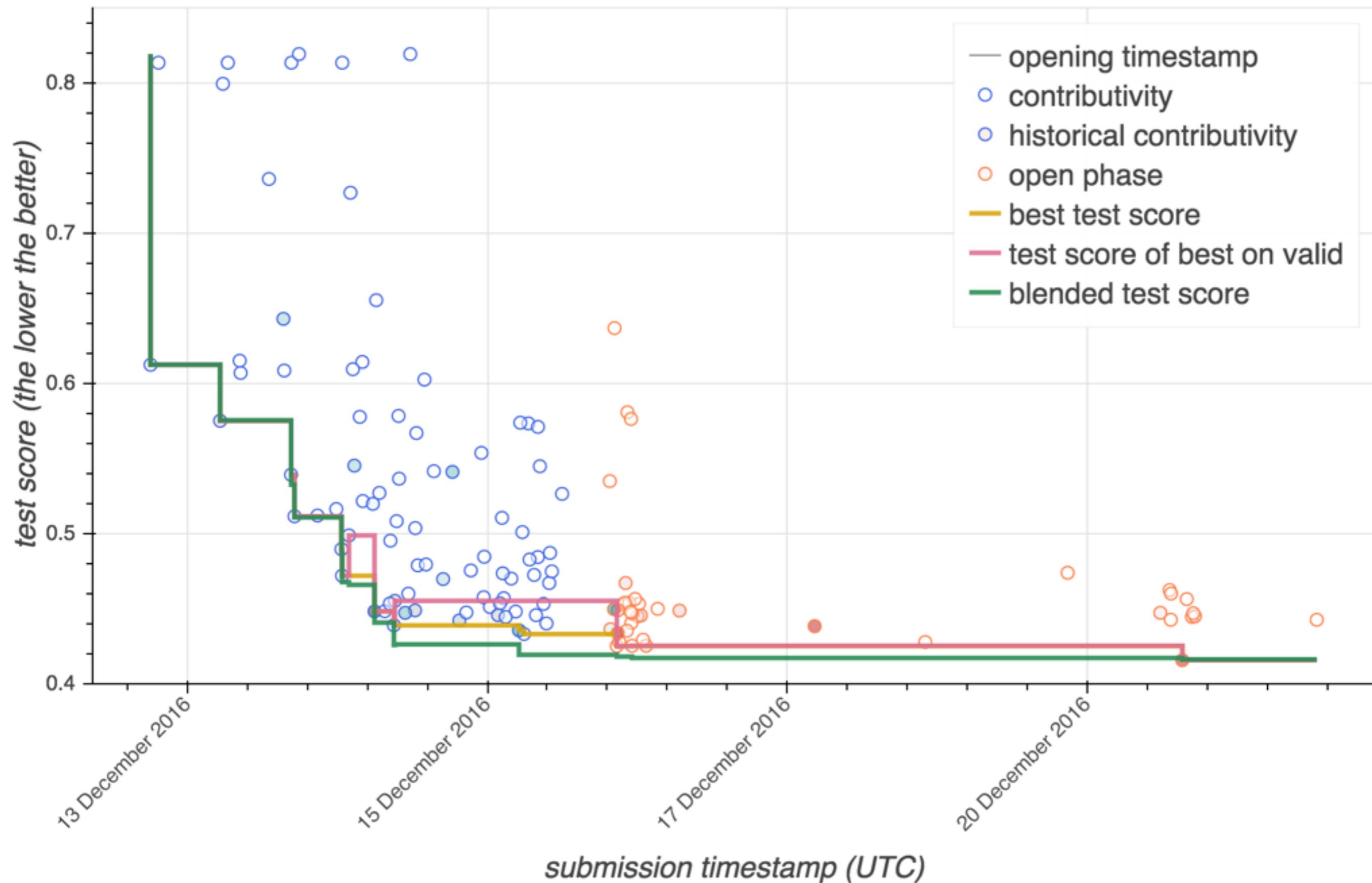
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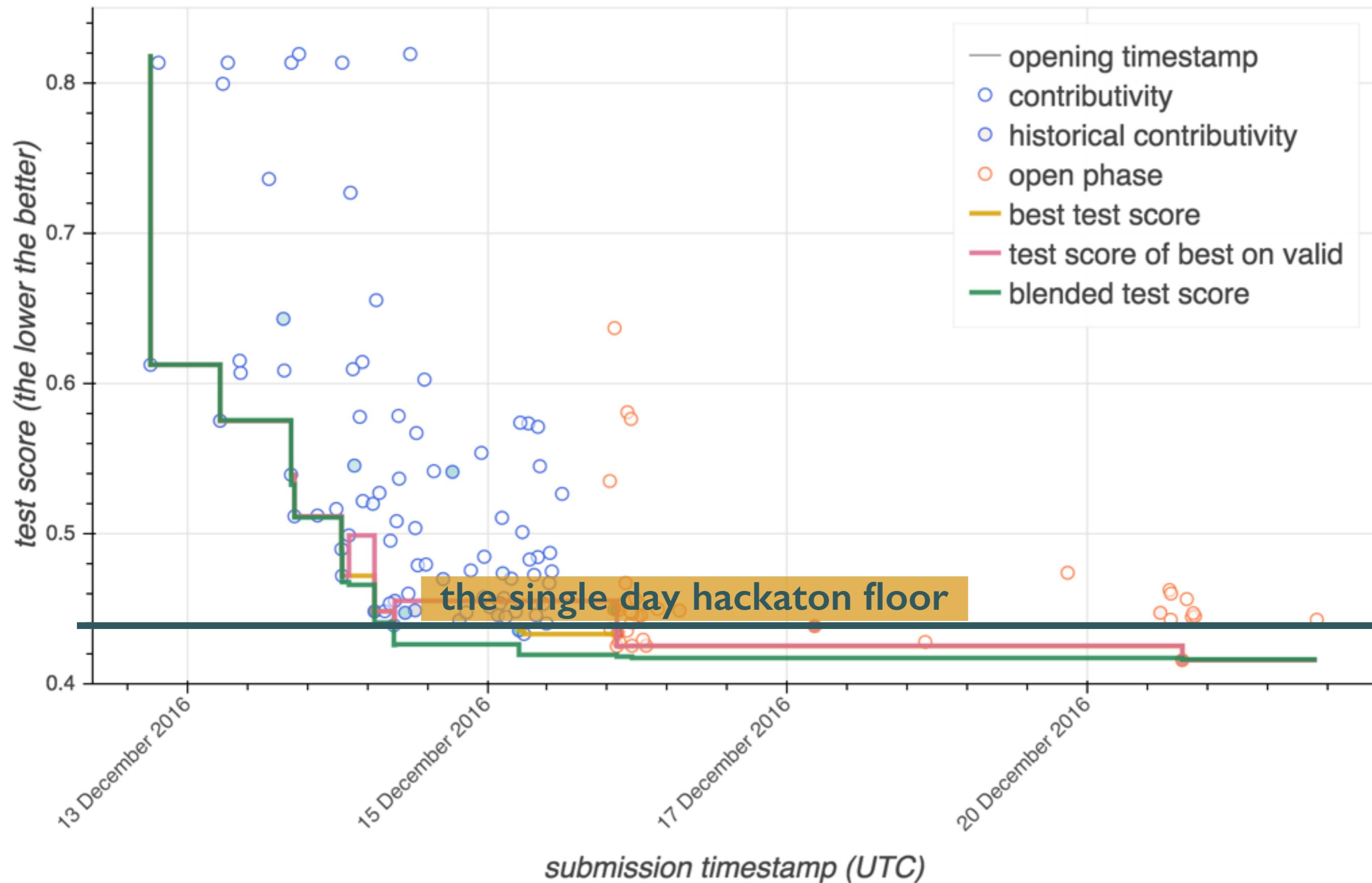
Hep detector anomalies test scores



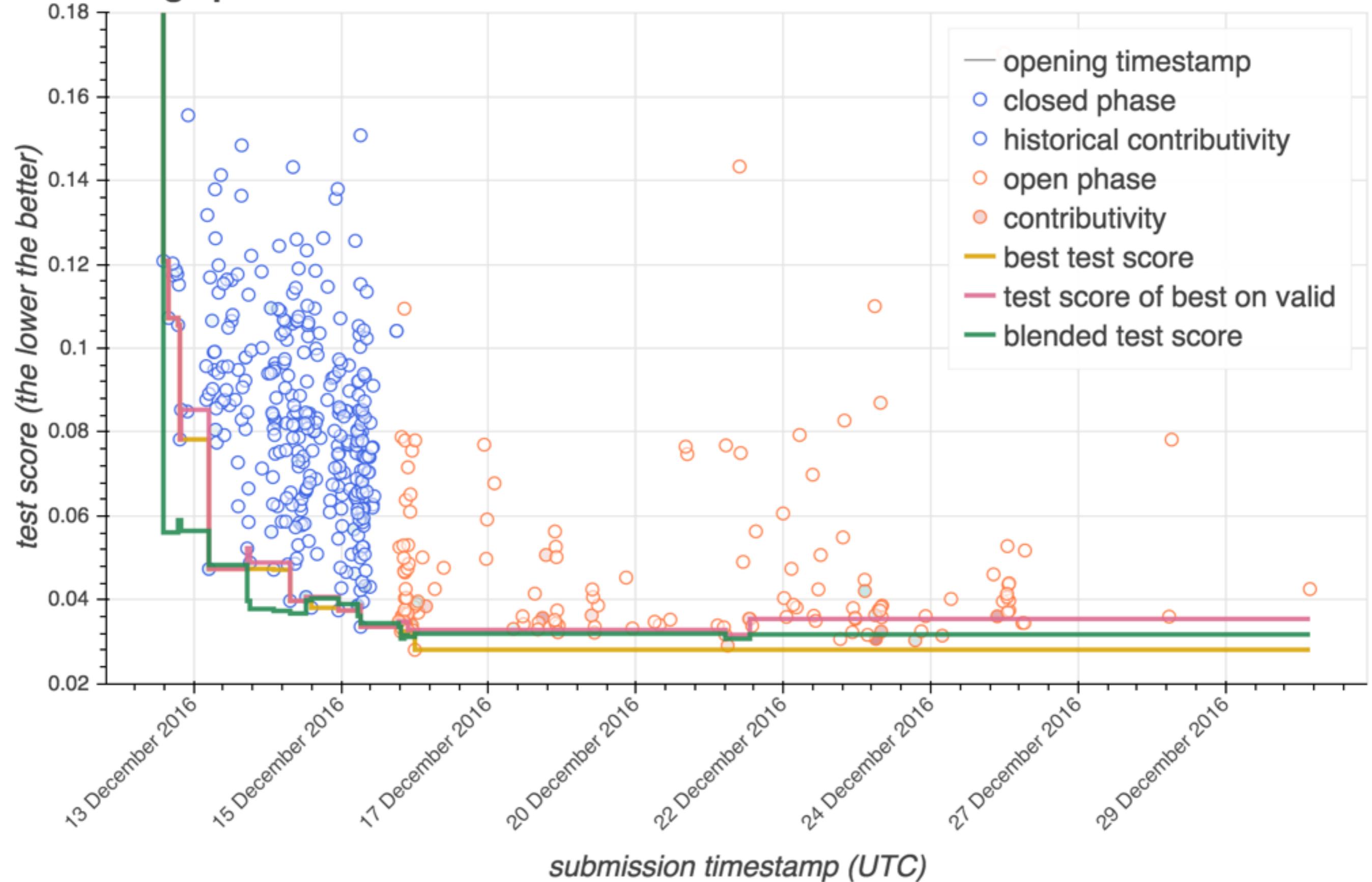
El nino forecast test scores



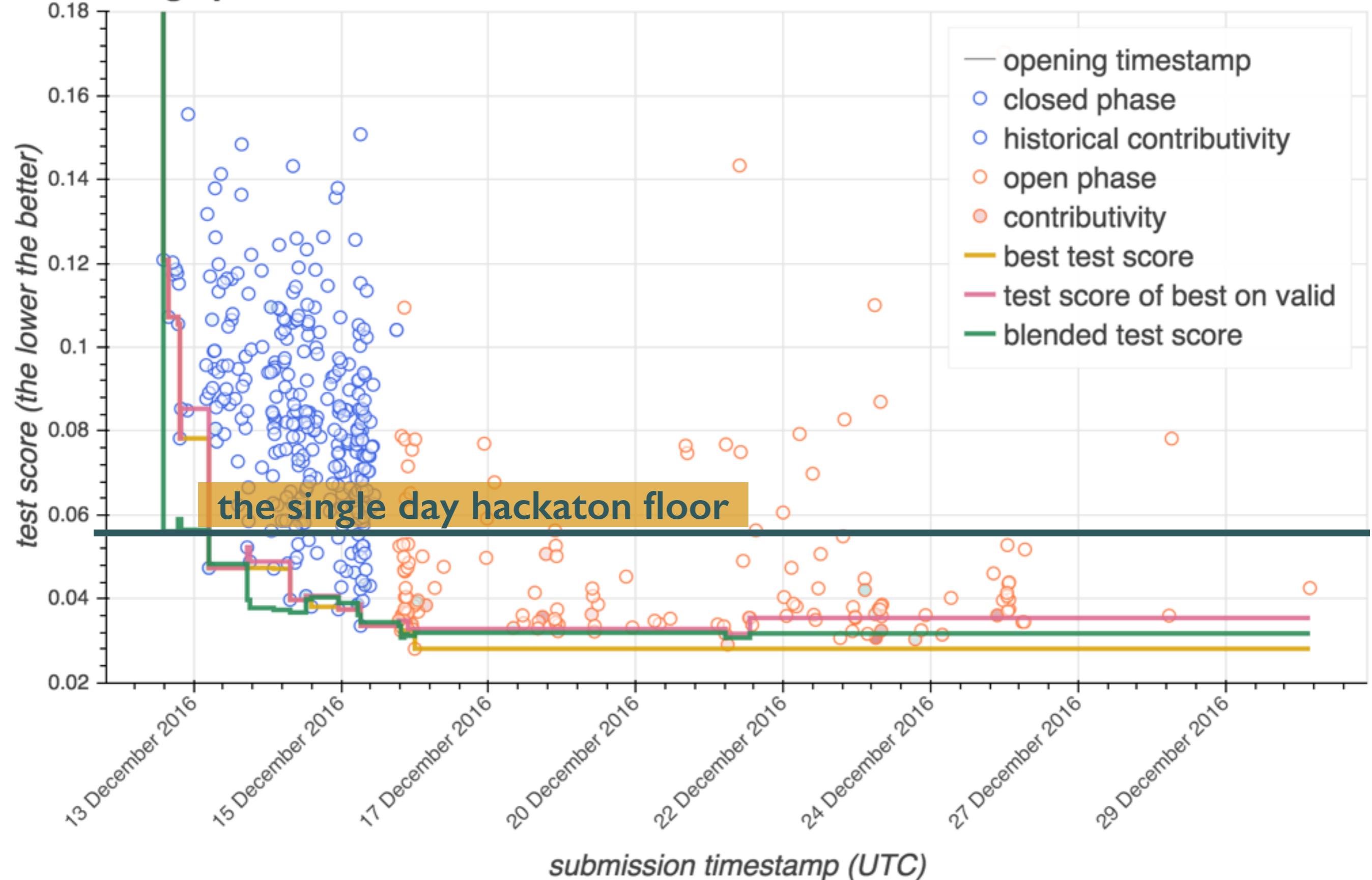
El nino forecast test scores



Drug spectra test scores



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WHAT WE LEARNED

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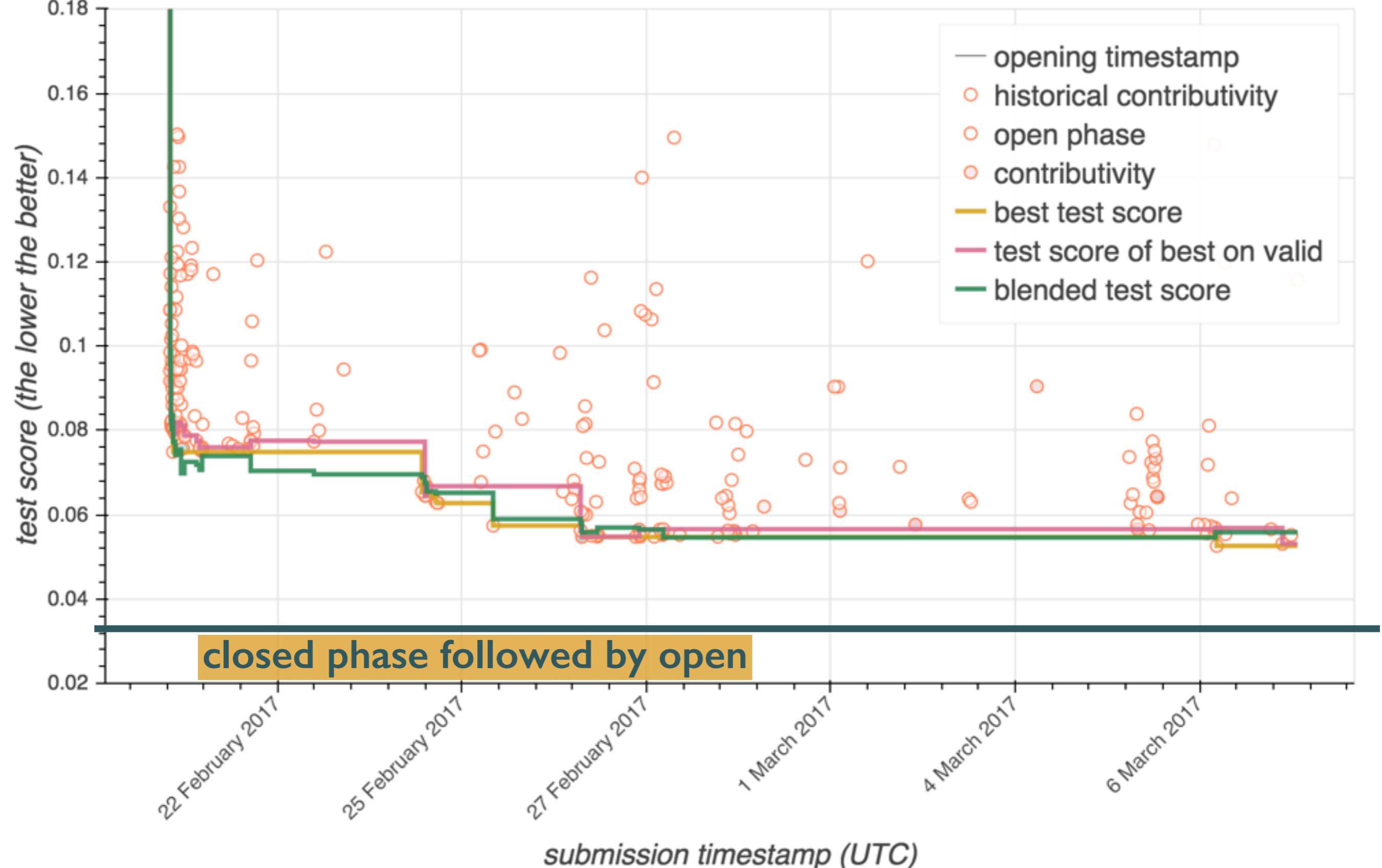
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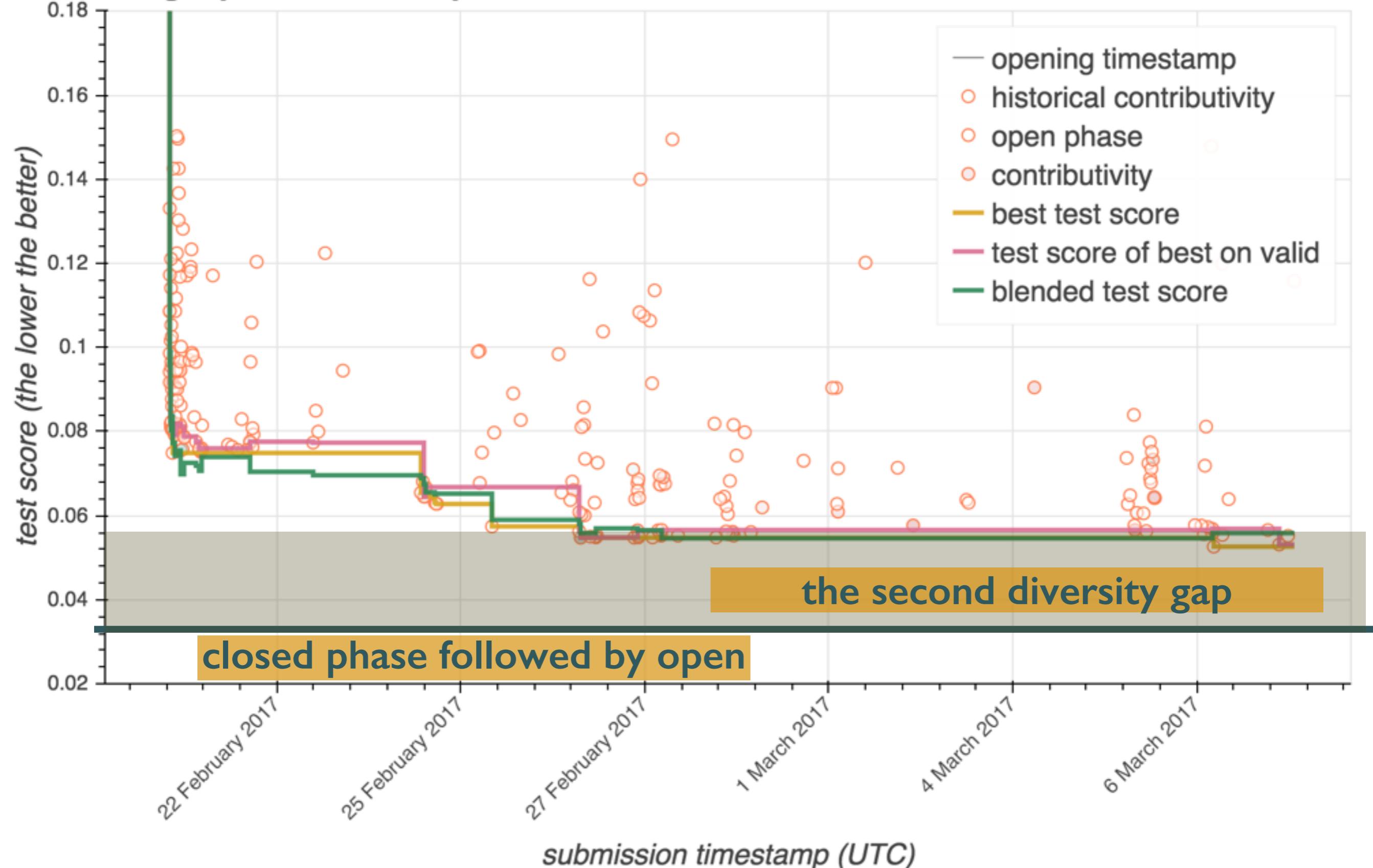
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- Course RAMPs beat single day hackatons significantly
 - larger number of students?
 - longer RAMPs?
 - novice and master-level students are better than data science researchers?
 - stronger incentives?
 - closed phase preceding an open phase (vs pure open RAMP) helps to create diversity?

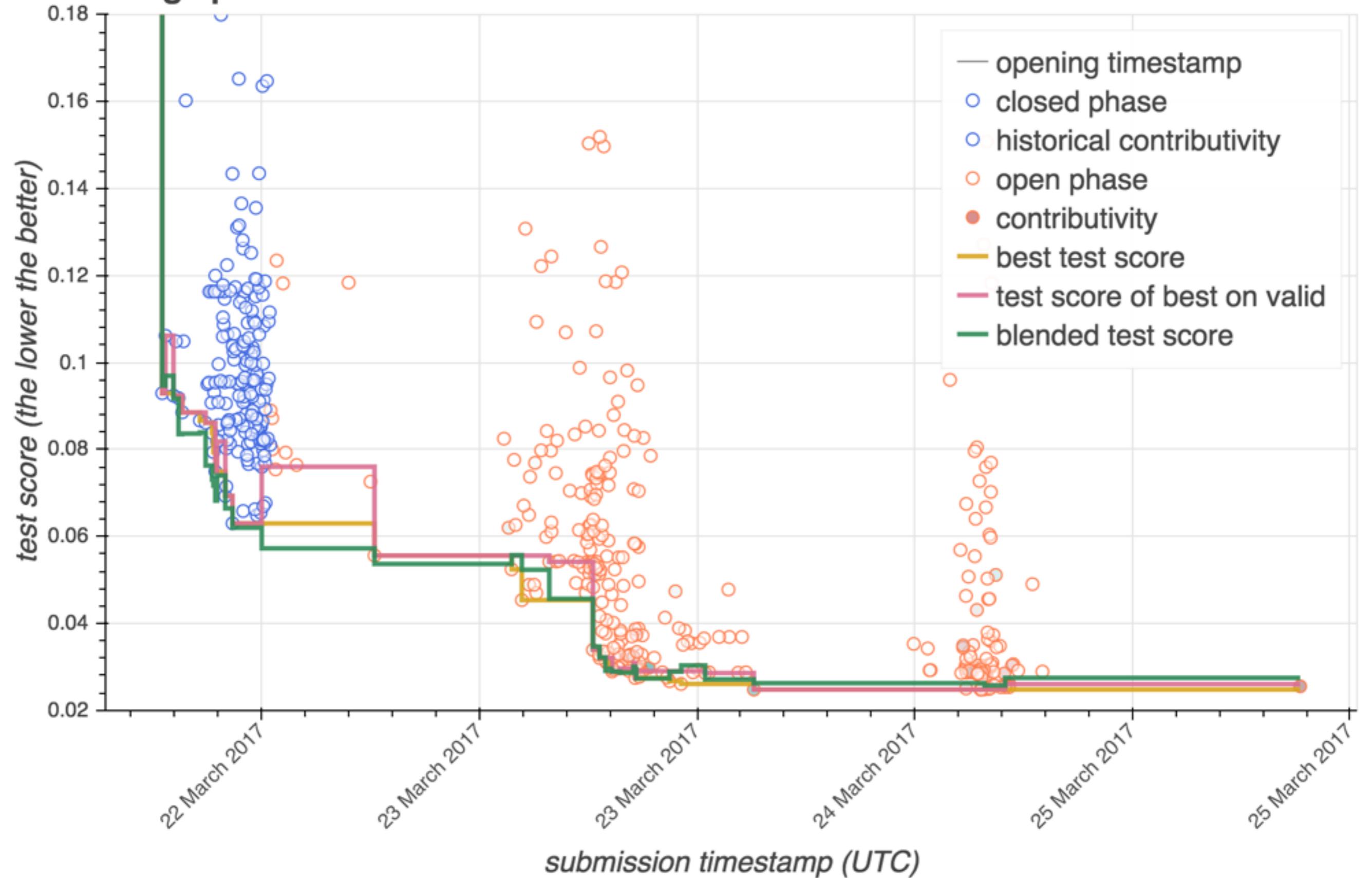
Drug_spectra_m1xmap583_201617 test scores



Drug_spectra_m1xmap583_201617 test scores



Drug spectra mines 2016/17 test scores



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

WHAT'S NEXT

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- More RAMPs
 - **galaxy** morphology, detecting **autism** from brain fMRI, detecting **Mars craters**, forecasting **space weather** (solar storm early warning)

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- Build your own RAMPs

WHAT IS IN IT FOR YOU

- If you are a **data science teacher**
 - we have been using **classroom RAMPs in different formats**: homework, final project, data camp
 - students **love it and work their butt off**, they **learn from each other** and **collaborate**
- If you are a **domain science researcher or data scientist**
 - We can **solve your predictive problems** better than any single researcher in a classical project
- If you are a **data science researcher or engineer**
 - You can **benchmark your new techniques** on a variety of problems

sign up: www.ramp.studio

contact us: balazs.kegl@gmail.com