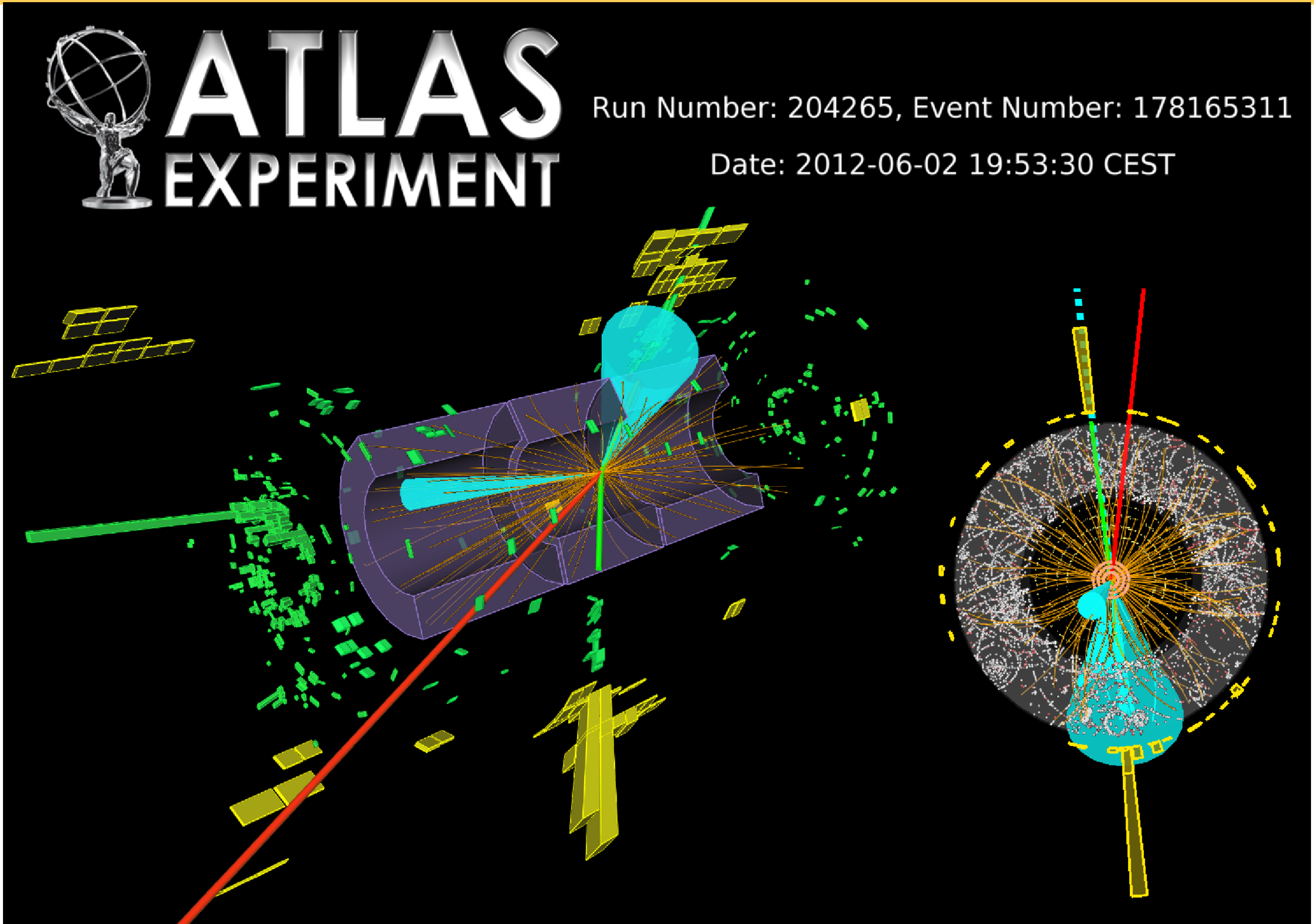
Introduction to the HEPML workshop and the HiggsML challenge

Balázs Kégl
David Rousseau, Cécile Germain, Isabelle Guyon, Glen Cowan

CNRS/IN2P3/University Paris-S{ud,aclay}, ChaLearn, Royal Holloway

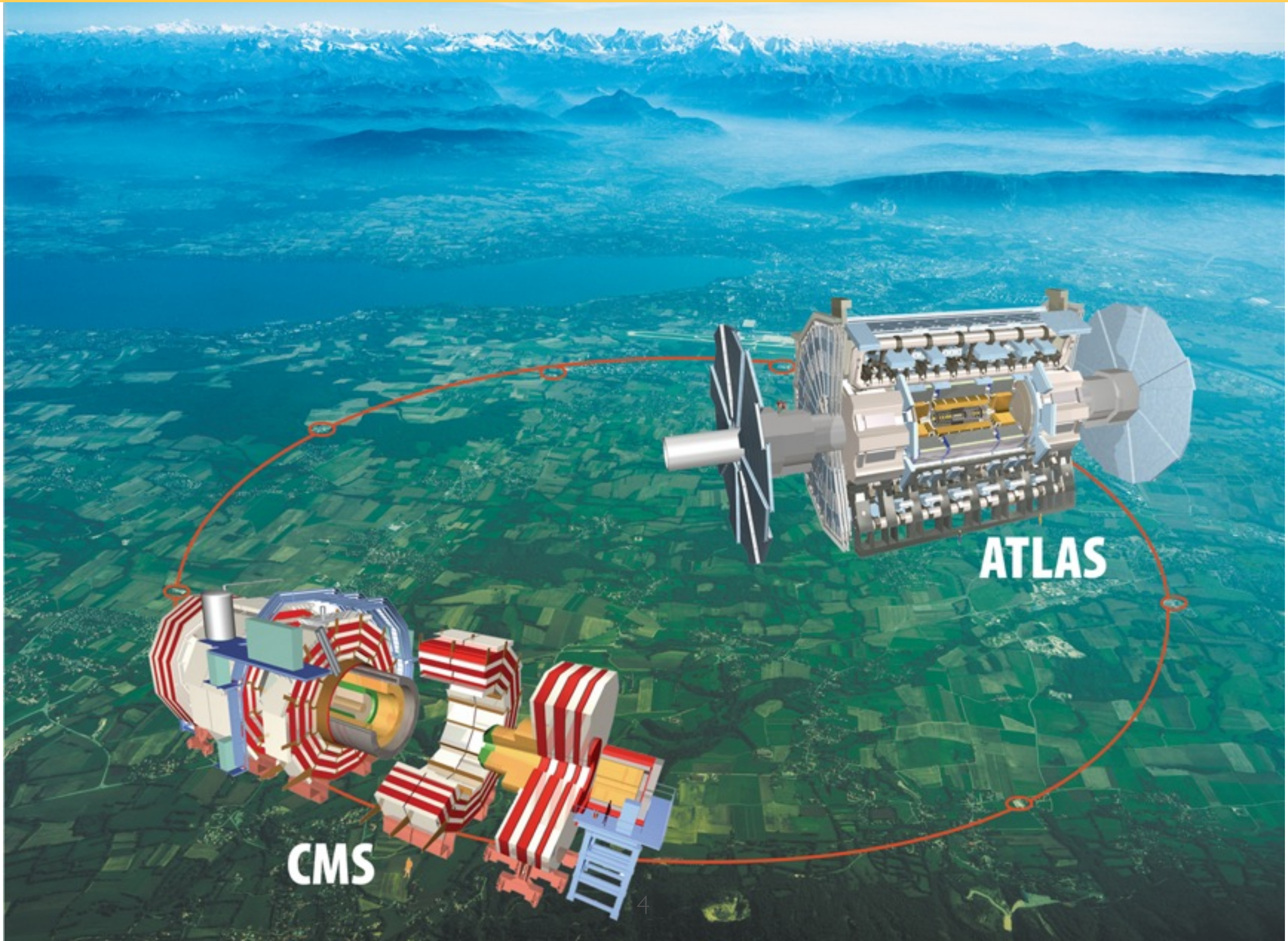
HEPML NIPS'14 workshop
December 13, 2014

Classification for discovery
The HiggsML challenge

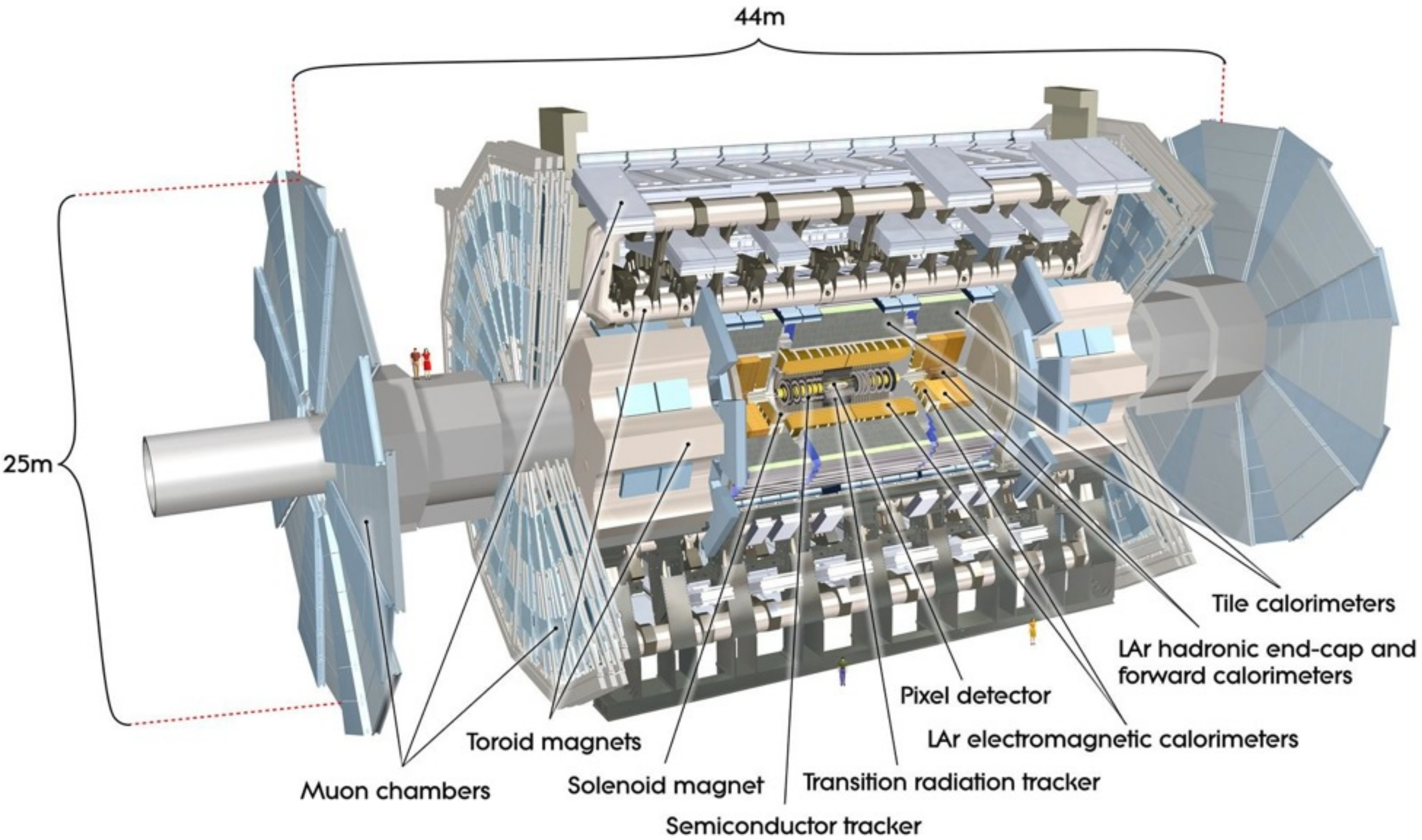

ATLAS EXPERIMENT
Run Number: 204265, Event Number: 178165311
Date: 2012-06-02 19:53:30 CEST

Data collection

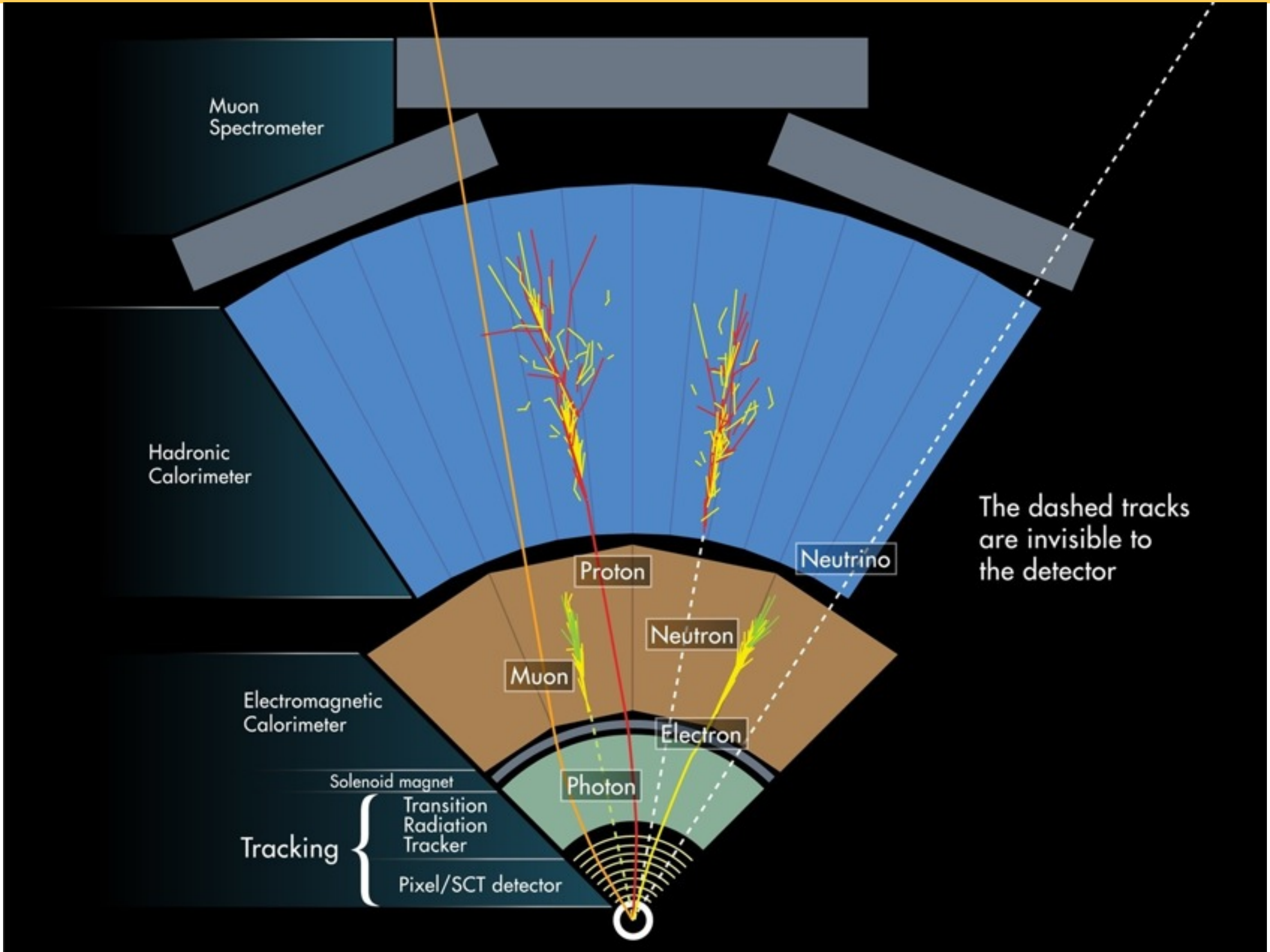
The LHC in Geneva



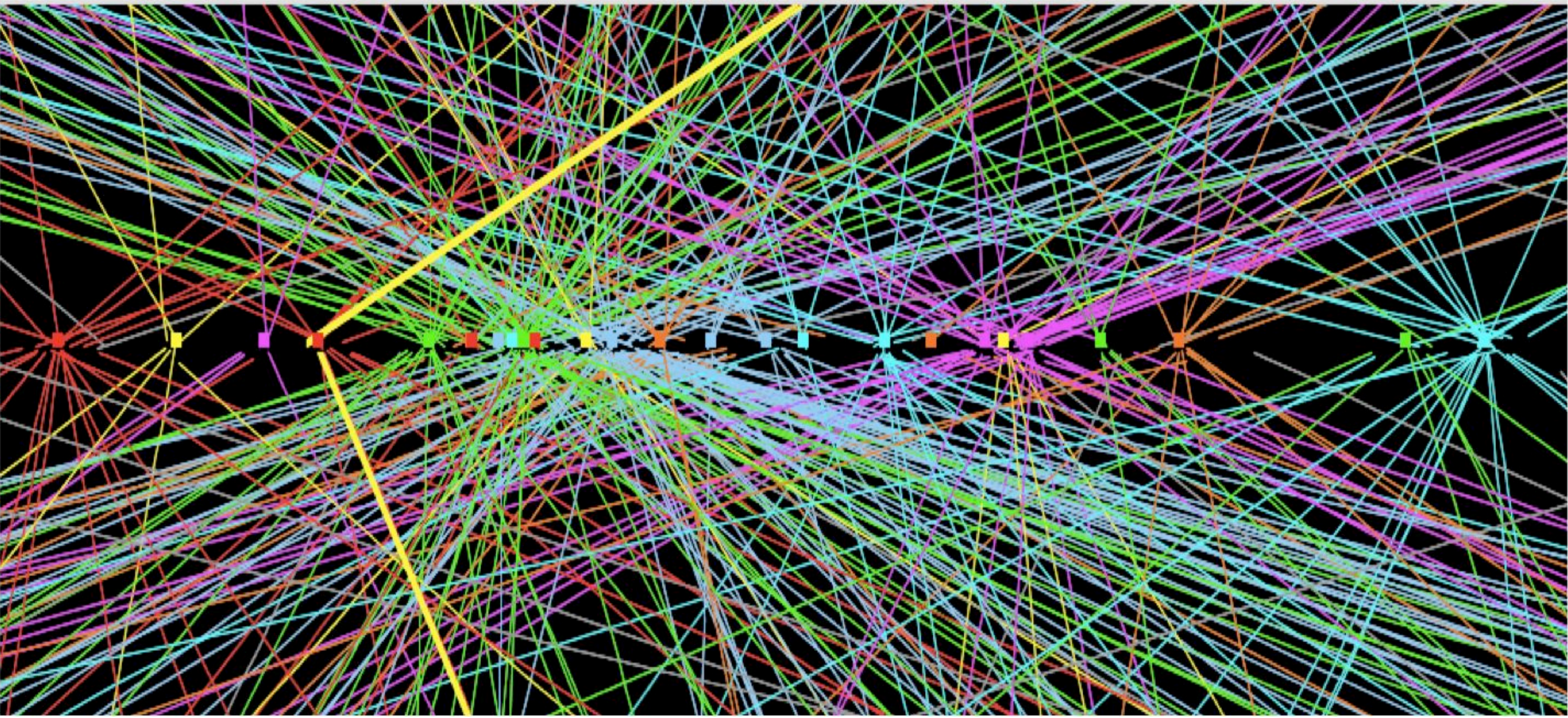
The ATLAS detector


44m
25m
Tile calorimeters
LAr hadronic end-cap and forward calorimeters
Pixel detector
LAr electromagnetic calorimeters
Toroid magnets
Muon chambers
Solenoid magnet
Transition radiation tracker
Semiconductor tracker

THE ATLAS DETECTOR



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

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

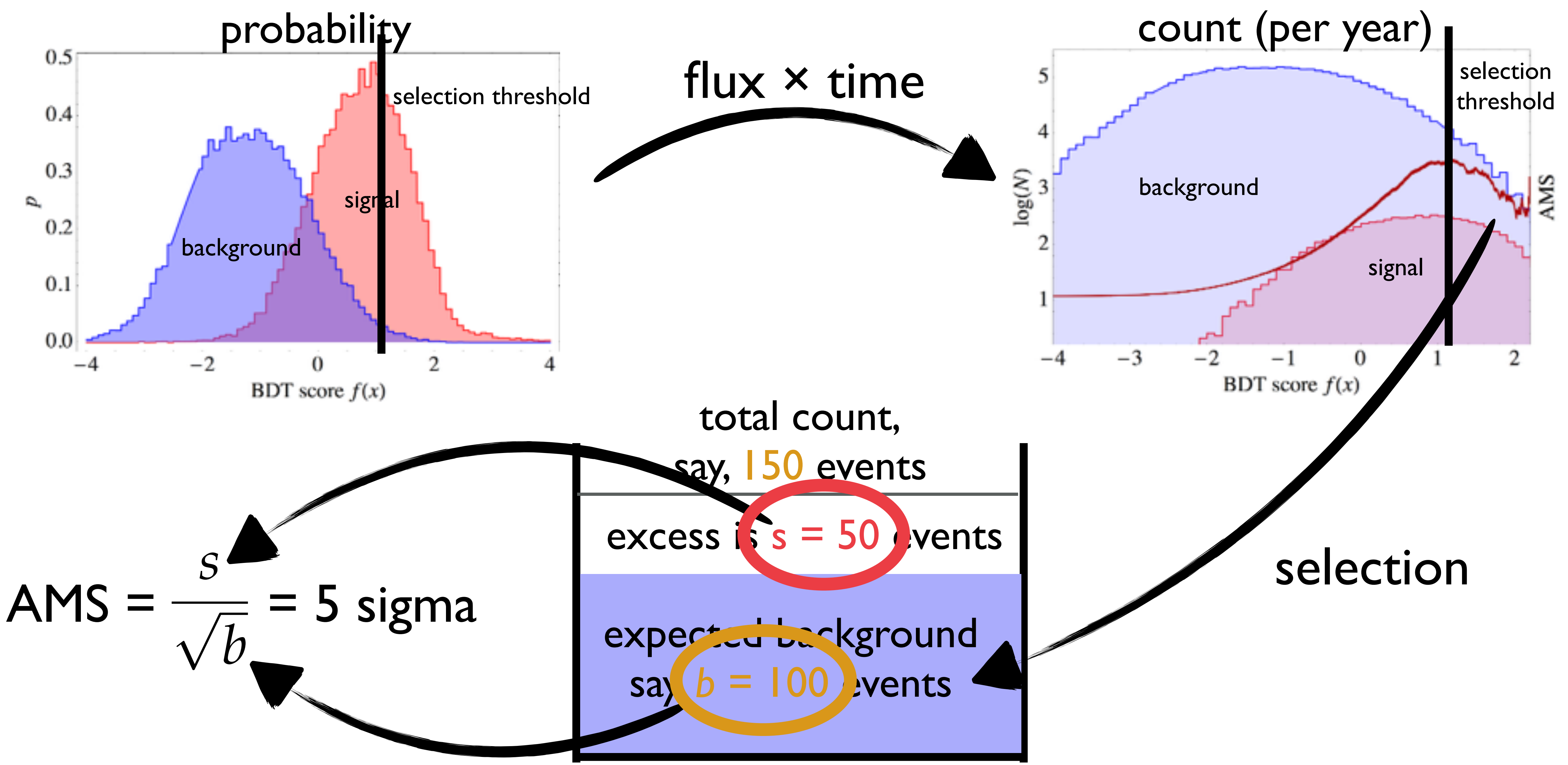
THE HIGGS TO TAU-TAU CHANNEL

- Highly **unbalanced** data
  - we expect to see **<100** Higgs bosons per year in $\approx 10^{10}$ events
  - after pre-selection, we will have
    500K **background (negative)** and
    1K **signal (positive)** events per year (2012)
  - Training on **simulated data**

The metric

Classification for discovery

Goal: optimize the expected discovery significance



probability

flux × time

count (per year)

selection

total count, say, 150 events

excess is s = 50 events

expected background say, b = 100 events

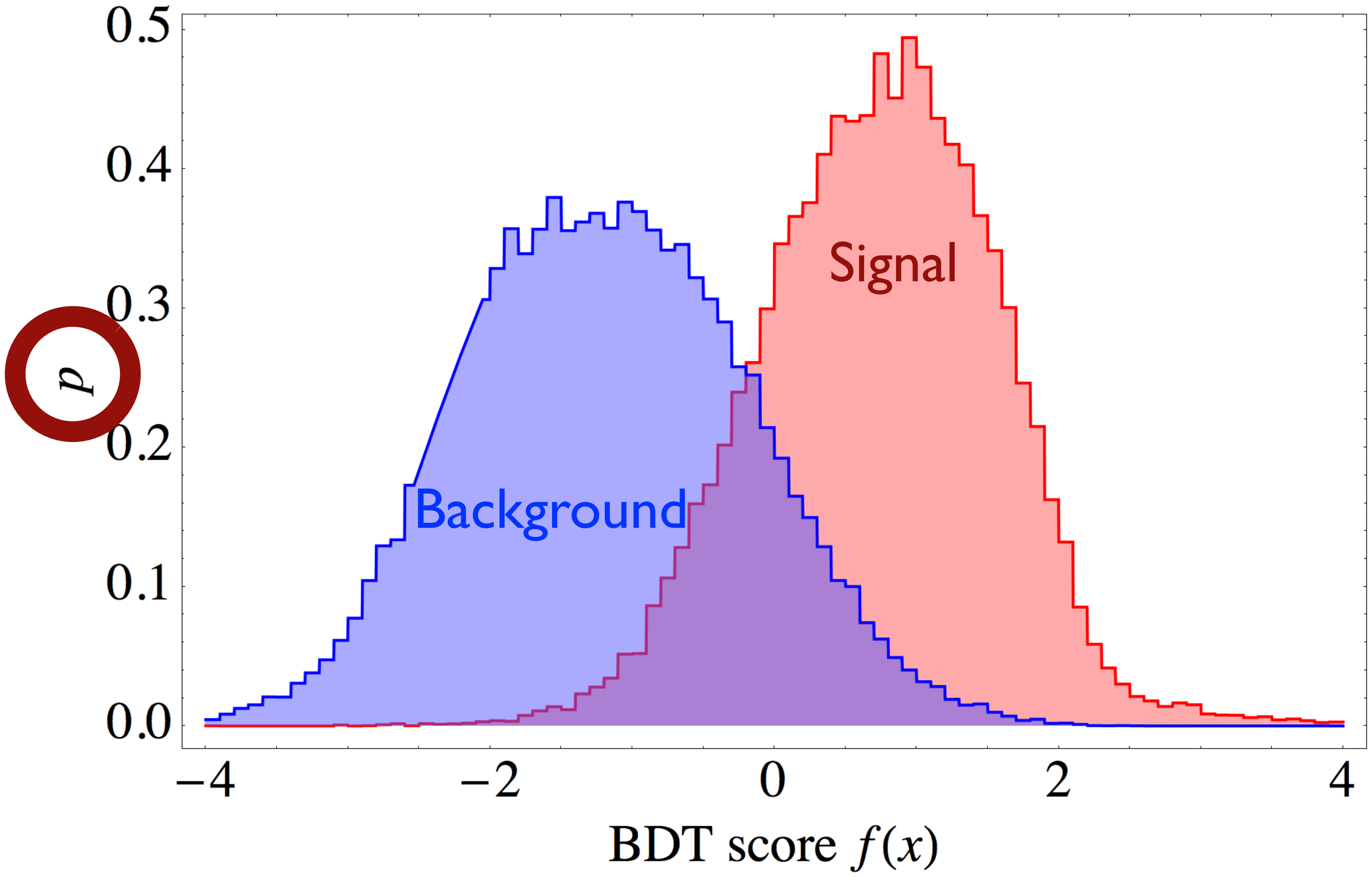
$$\text{AMS} = \frac{s}{\sqrt{b}} = 5 \text{ sigma}$$

CLASSIFICATION FOR DISCOVERY

How to design g to maximize the sensitivity?

- A two-stage approach

  1. optimize a discriminant (score) function $f : \mathbb{R}^d \to \mathbb{R}$ using a classical learning algorithm (BDT, NN)



Classification for discovery

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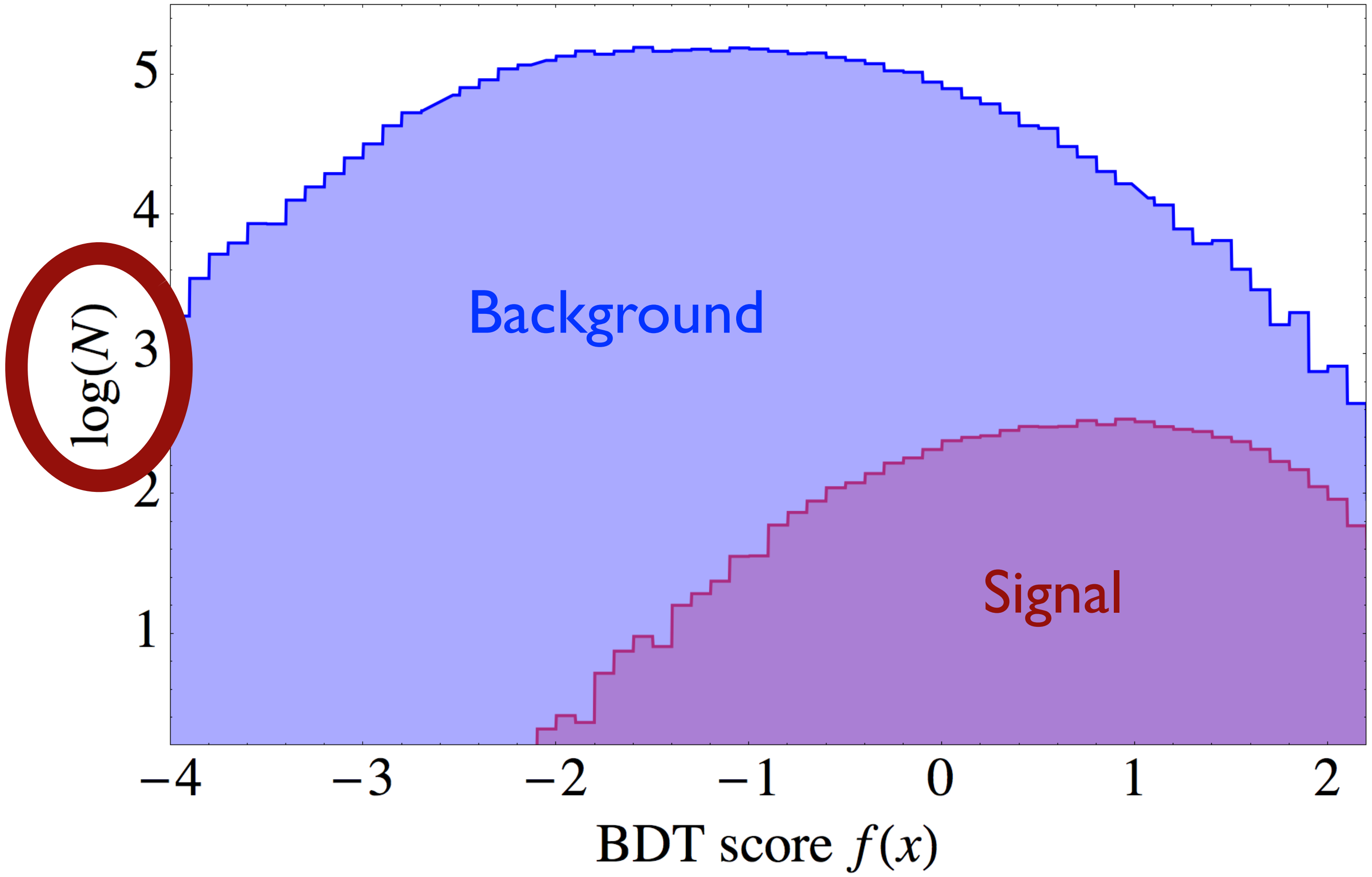

CLASSIFICATION FOR DISCOVERY

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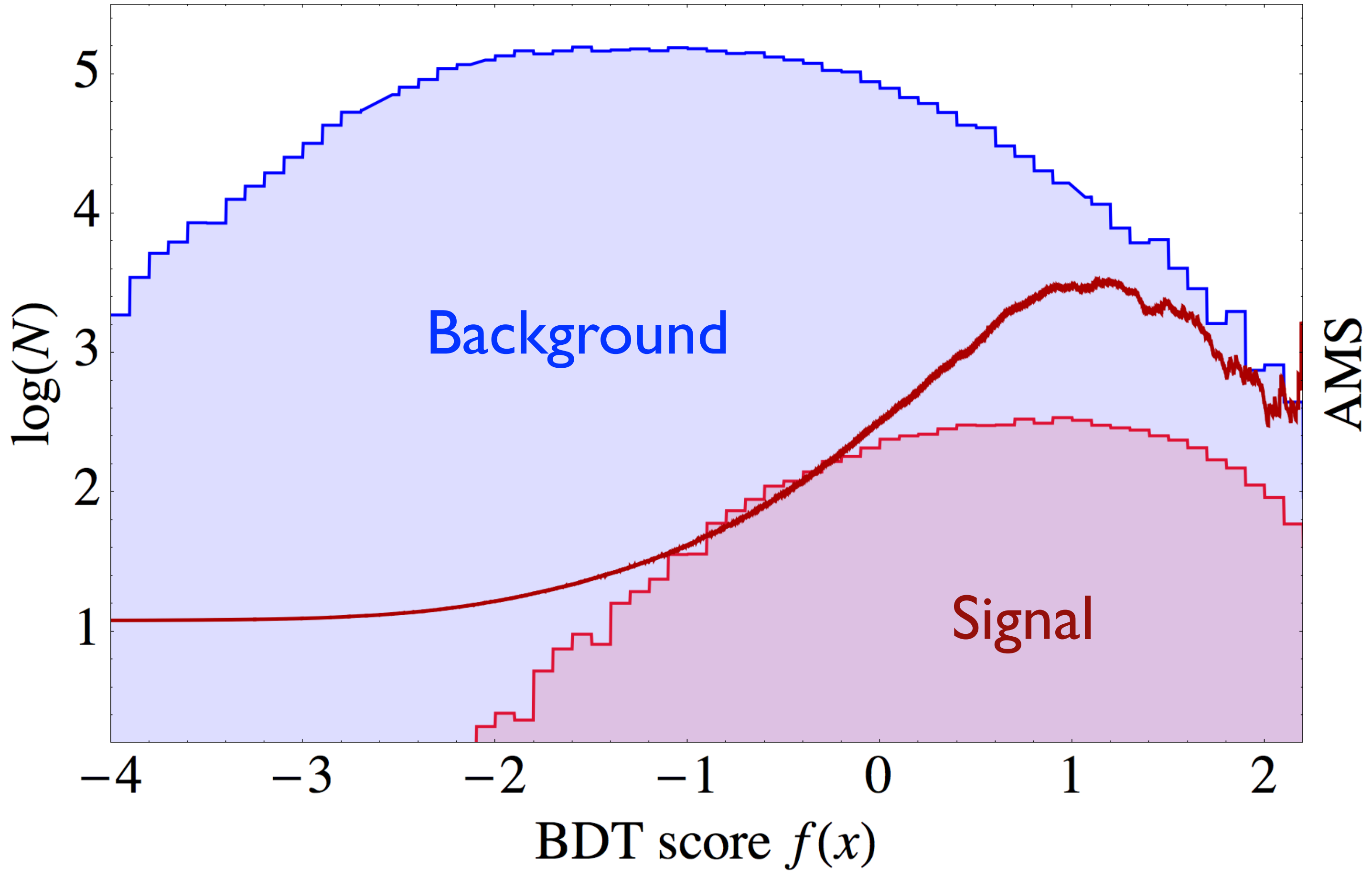
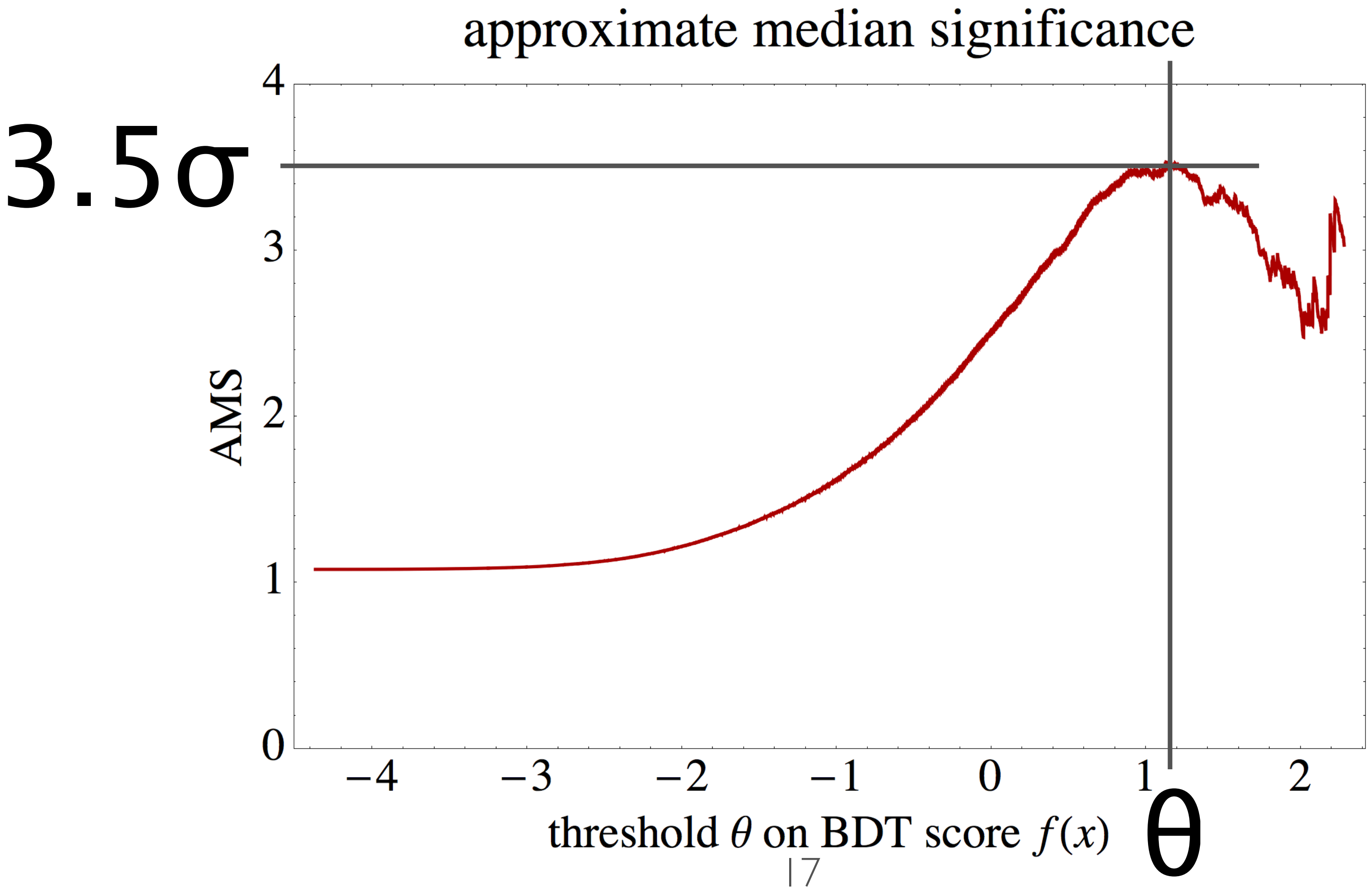


CLASSIFICATION FOR DISCOVERY

How to design g to maximize the sensitivity?

- A two-stage approach (make figure with score)

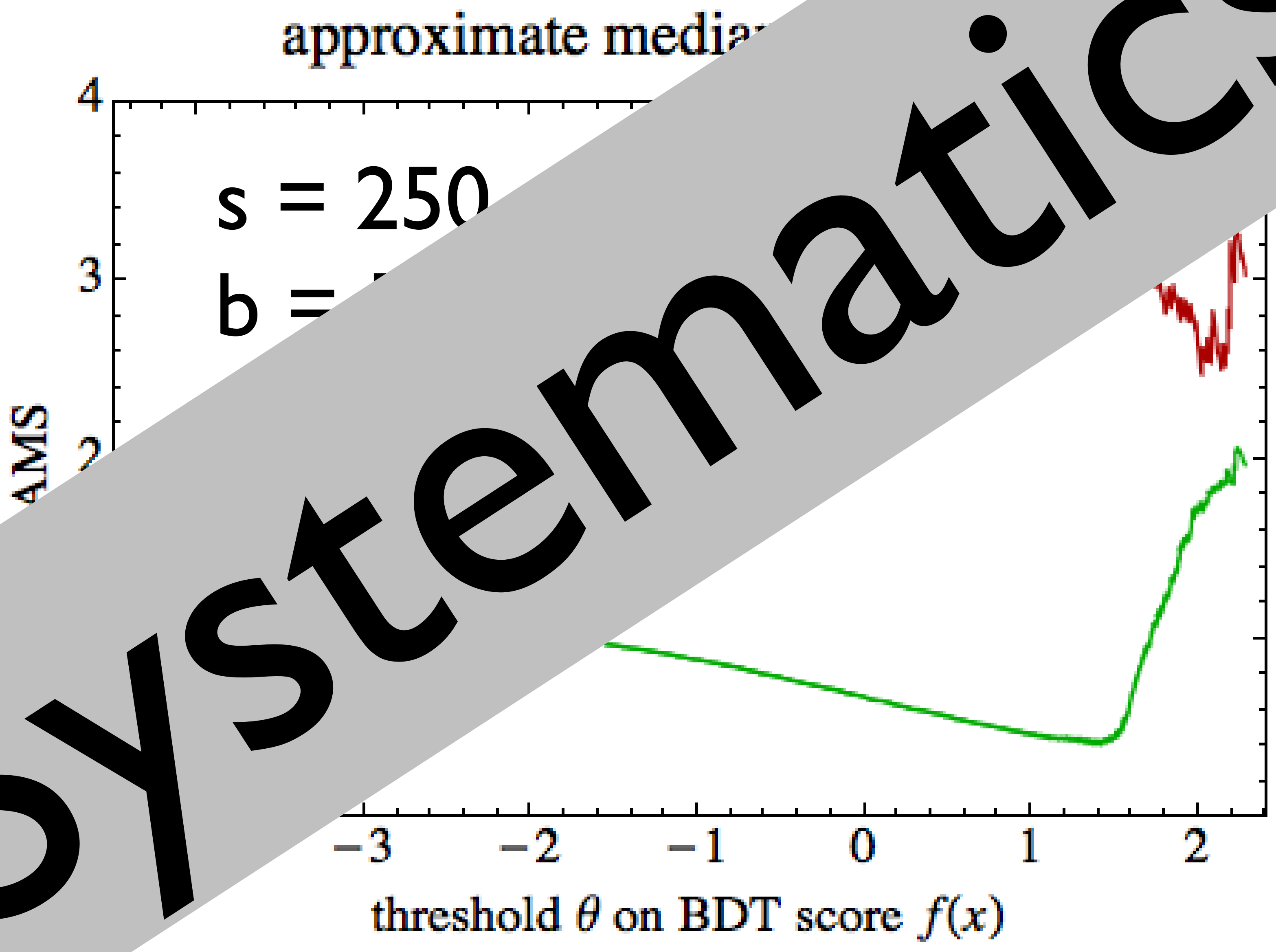
1. optimize a discriminant (score) function $f : \mathbb{R}^d \to \mathbb{R}$ using a classical learning algorithm (BDT, NN)
2. define $g(\mathbf{x}) = \text{sign}\big(f(\mathbf{x}) - \theta\big)$ and optimize θ for maximizing the AMS



Classification for discovery

Comparing with Atlas analysis

- Atlas does a manual pre-selection (category), th of the AMS is completely eliminated. Why?



Systematics!

CLASSIFICATION FOR DISCOVERY

How to handle systematic (model) uncertainties?

- OK, so let's design an objective function that can take background systematics into consideration

  - Likelihood with unknown background $b \sim \mathcal{N}(\mu_\mathsf{b}, \sigma_\mathsf{b})$

$$L(\mu_\mathsf{s}, \mu_\mathsf{b}) = P(n, b | \mu_\mathsf{s}, \mu_\mathsf{b}, \sigma_\mathsf{b}) = \frac{(\mu_\mathsf{s} + \mu_\mathsf{b})^n}{n!} e^{-(\mu_\mathsf{s}+\mu_\mathsf{b})} \frac{1}{\sqrt{2\pi}\sigma_\mathsf{b}} e^{-(b-\mu_\mathsf{b})^2/2{\sigma_\mathsf{b}}^2}$$

  - Profile likelihood ratio $\lambda(0) = \frac{L(0, \hat{\hat{\mu}}_\mathsf{b})}{L(\hat{\mu}_\mathsf{s}, \hat{\mu}_\mathsf{b})}$

  - The new Approximate Median Significance (by Glen Cowan)

$$\mathsf{AMS} = \sqrt{2\left((s+b)\ln\frac{s+b}{b_0} - s - b + b_0\right) + \frac{(b-b_0)^2}{{\sigma_\mathsf{b}}^2}}$$

where

$$b_0 = \frac{1}{2}\left(b - {\sigma_\mathsf{b}}^2 + \sqrt{(b - {\sigma_\mathsf{b}}^2)^2 + 4(s+b){\sigma_\mathsf{b}}^2}\right)$$

Classification for discovery

How to handle systematic (model) uncertainties?

- The new Approximate Median Significance

$$\text{AMS} = \sqrt{2\left((s+b)\ln\frac{s+b}{b_0} - s - b + b_0\right) + \frac{(b-b_0)^2}{\sigma_\text{b}{}^2}}$$

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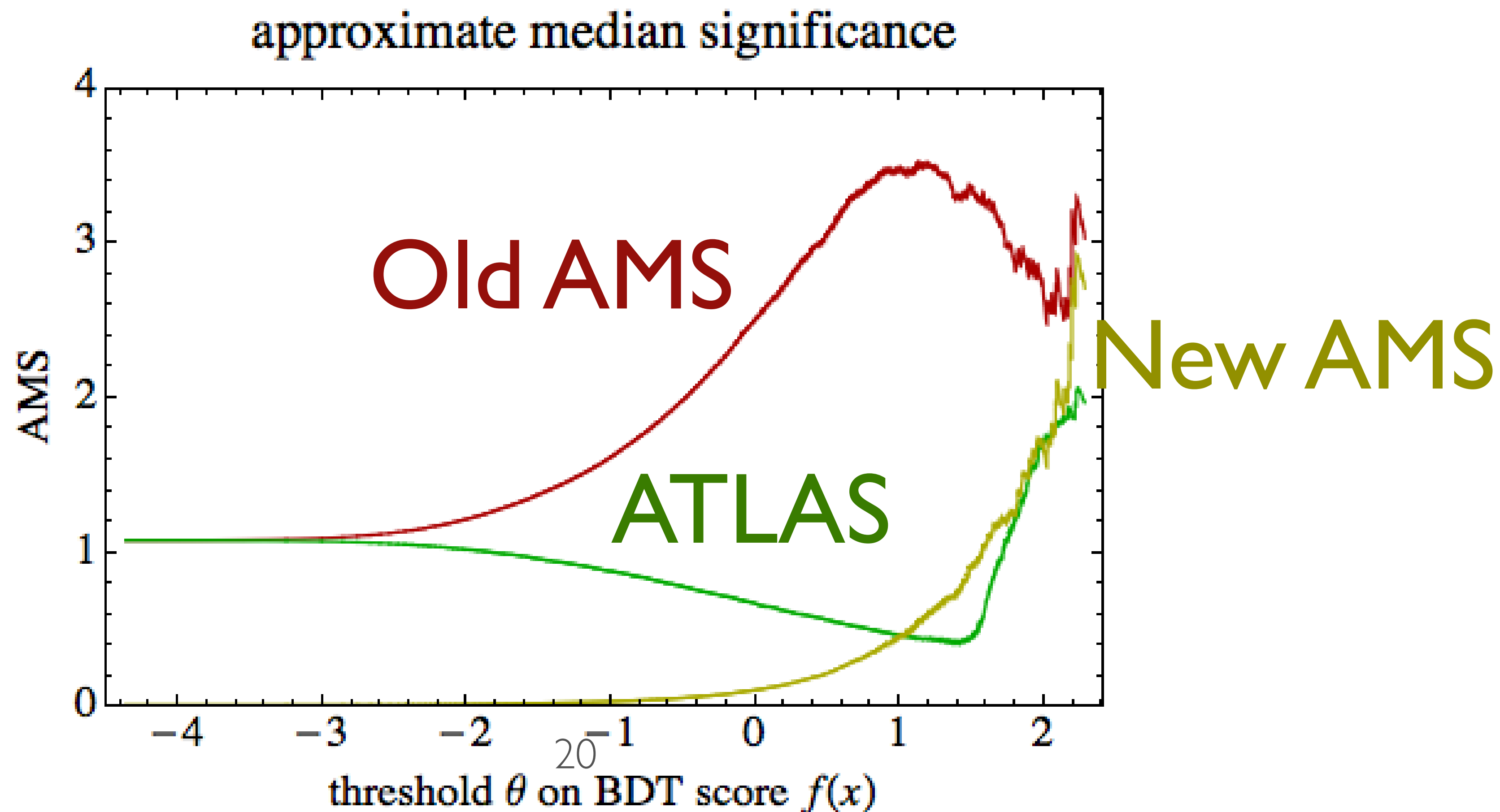
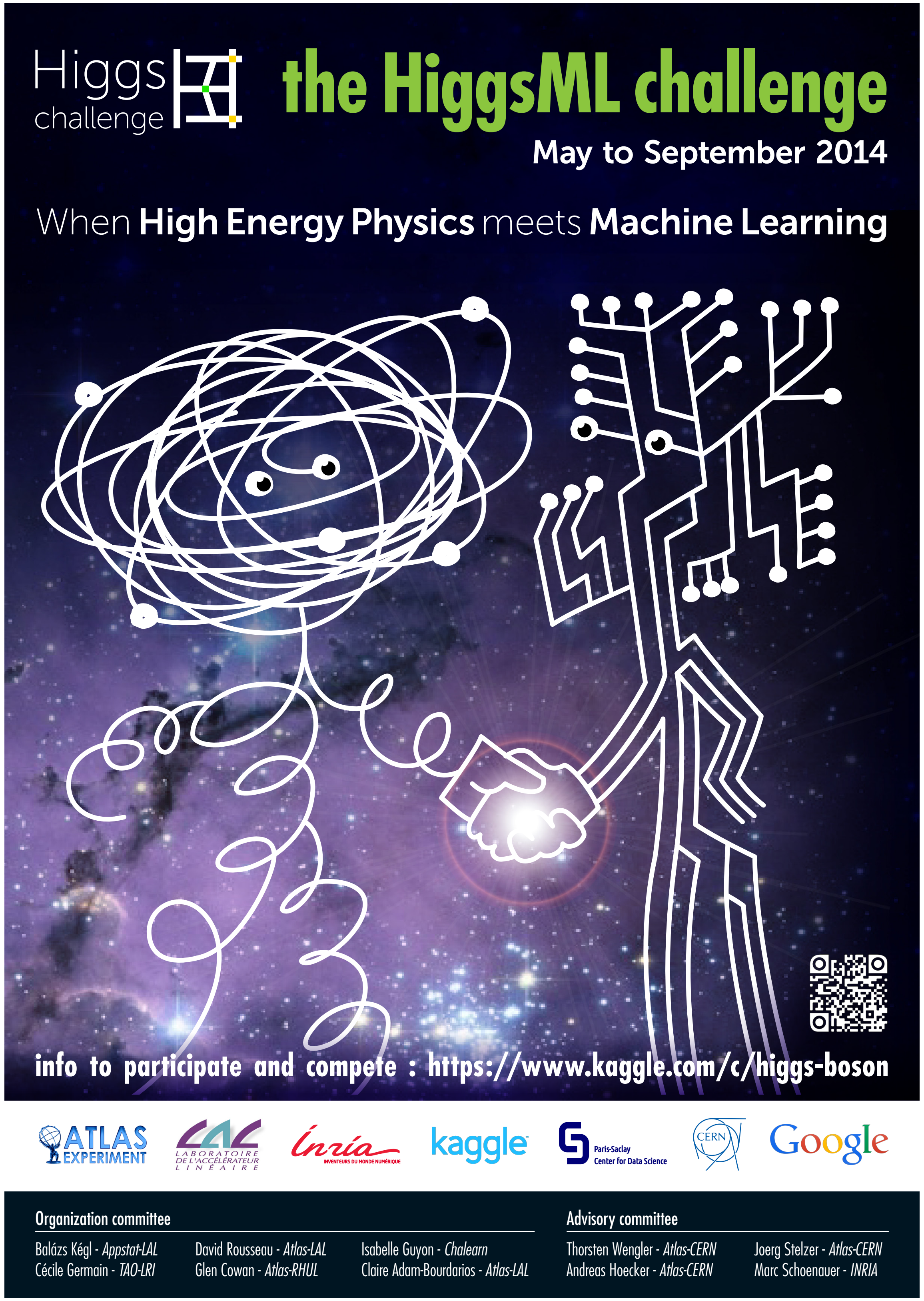


CLASSIFICATION FOR DISCOVERY

- Exciting physics
    - The Higgs to tau-tau excess is not yet at five sigma
      Tech. Rep. ATLAS-CONF-2013-108
- Exciting data science
    - What is the theoretical relationship between classification and test sensitivity?
    - What is the quantitative criteria to optimize?
    - How to formally include systematic uncertainties?
    - How to design (or redesign classical) algorithms for optimizing the criteria?
    - Redesign the counting test?

Classification for discovery

We organized a
data challenge
to answer some of these
questions



Higgs challenge

the HiggsML challenge

May to September 2014

When **High Energy Physics** meets **Machine Learning**

info to participate and compete : https://www.kaggle.com/c/higgs-boson

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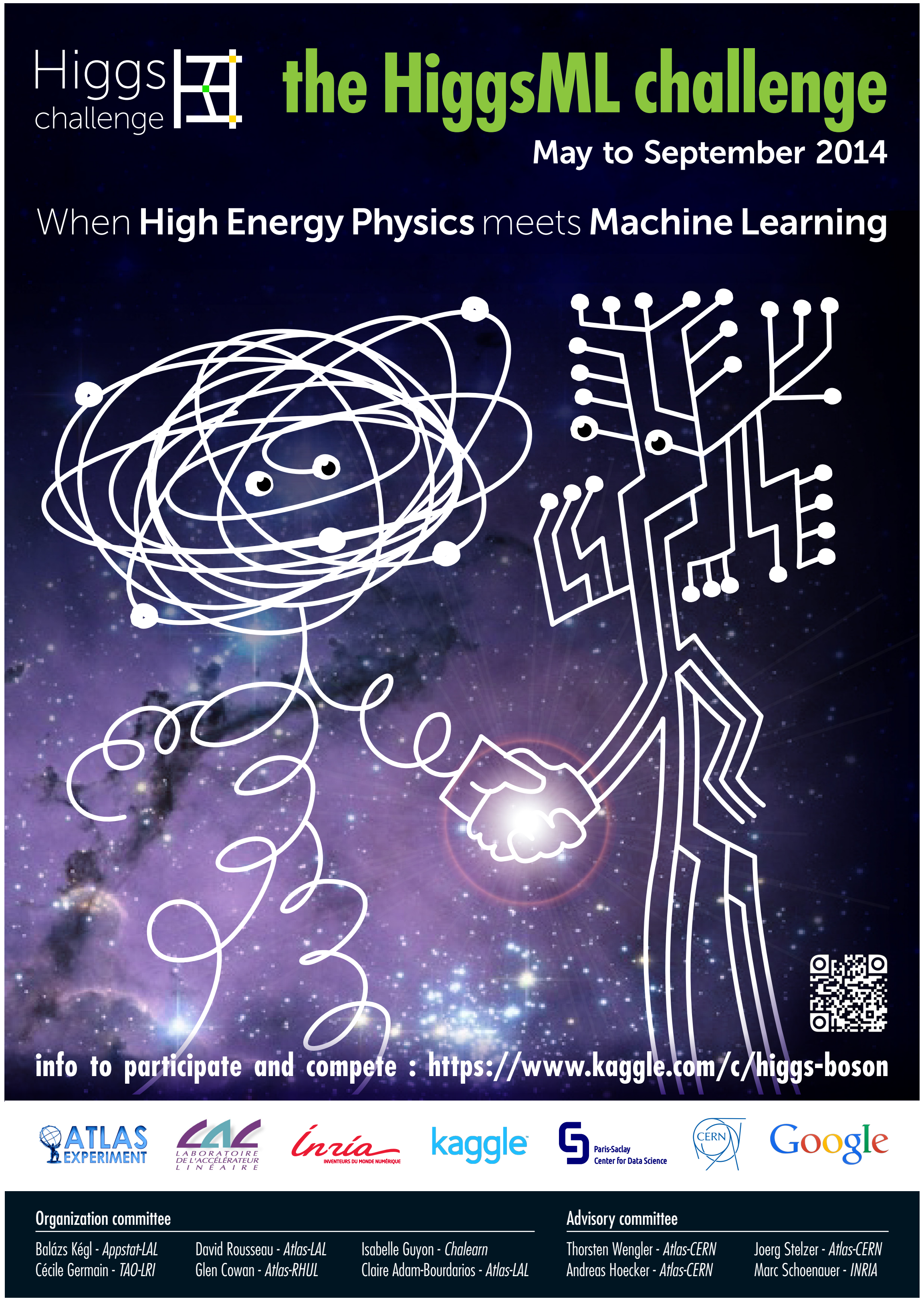
Marc Schoenauer - *INRIA*

Classification for Discovery

- Organizing committee
  - David Rousseau (ATLAS / LAL)
  - Balázs Kégl (AppStat / LAL)
  - Cécile Germain (LRI / UPSud)
  - Glen Cowan (ATLAS / Royal Holloway)
  - Claire Adam Bourdarios (ATLAS / LAL)
  - Isabelle Guyon (ChaLearn)



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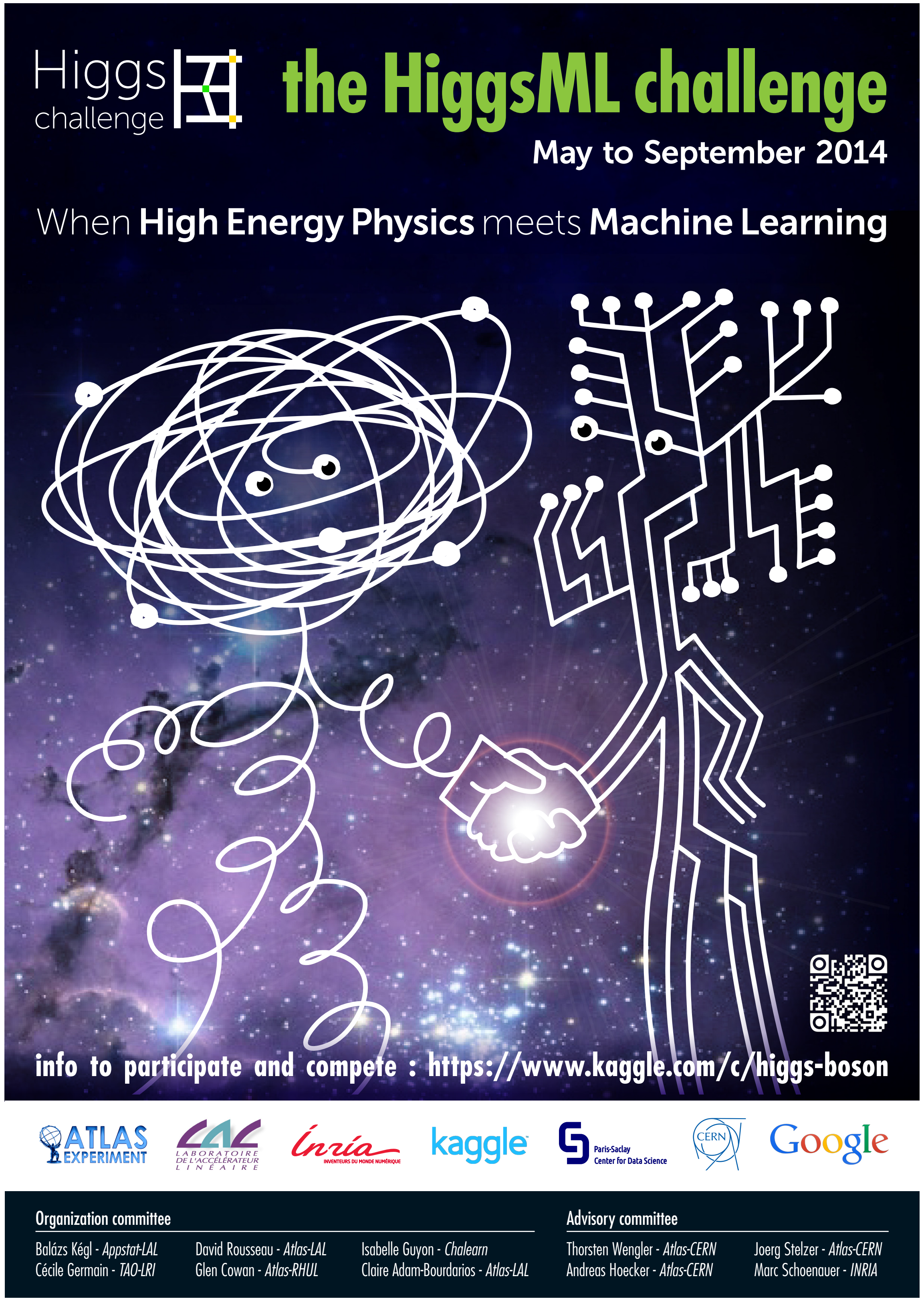
Classification for discovery

- 16K$ prize pool
  - 7-4-2K$ for the top three
  - HEP meets ML award for the most useful model, decided by the ATLAS members of the organizing committee



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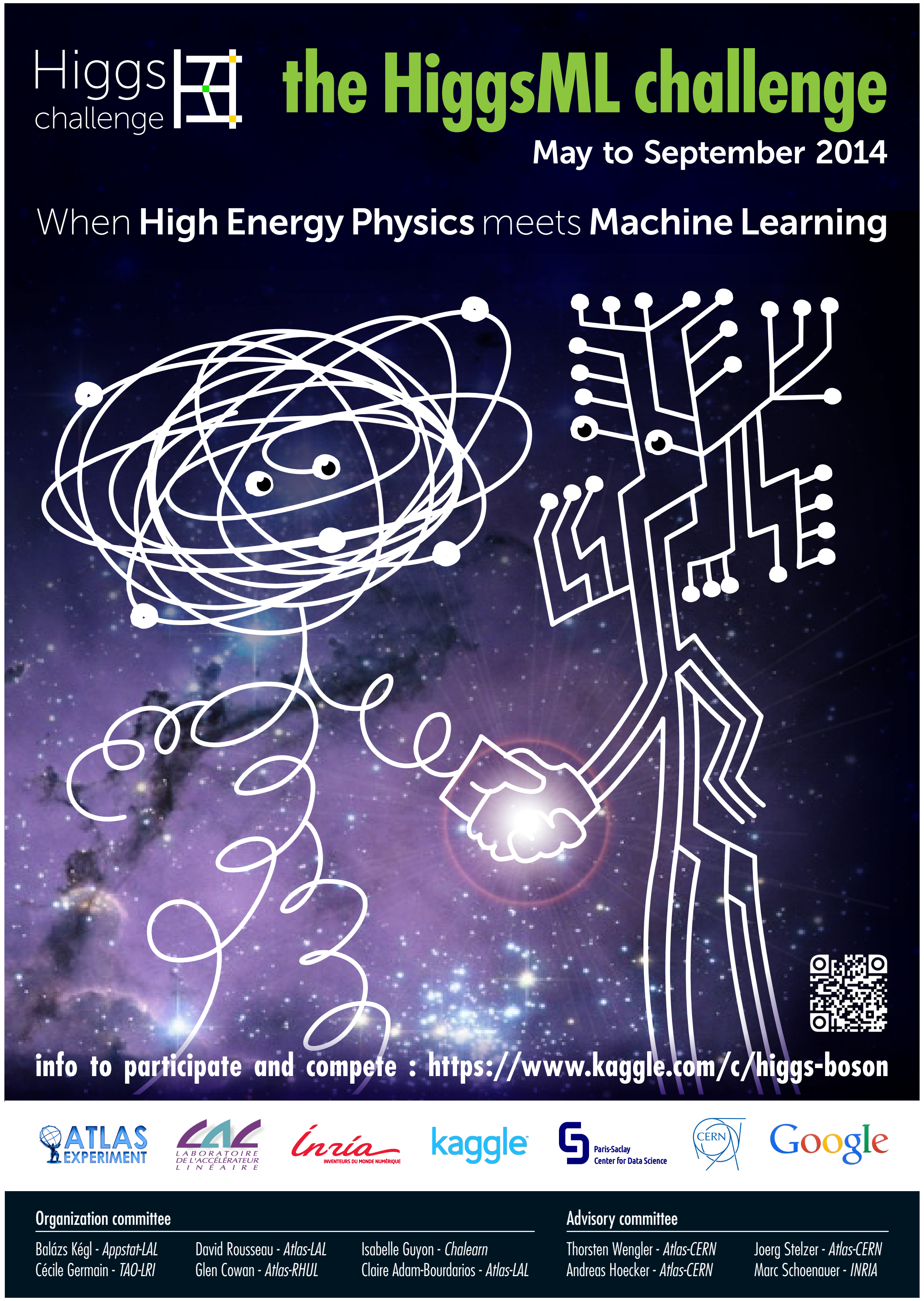
CLASSIFICATION FOR DISCOVERY

- Official ATLAS GEANT4 simulations
  - 30 features (variables)
  - 250K training: input, label, weight
  - 100K public test (AMS displayed real-time), only input
  - 450K private test (to determine the winner after the closing of the challenge), only input
  - public and private tests are shuffled, participants submit a vector of 550K labels



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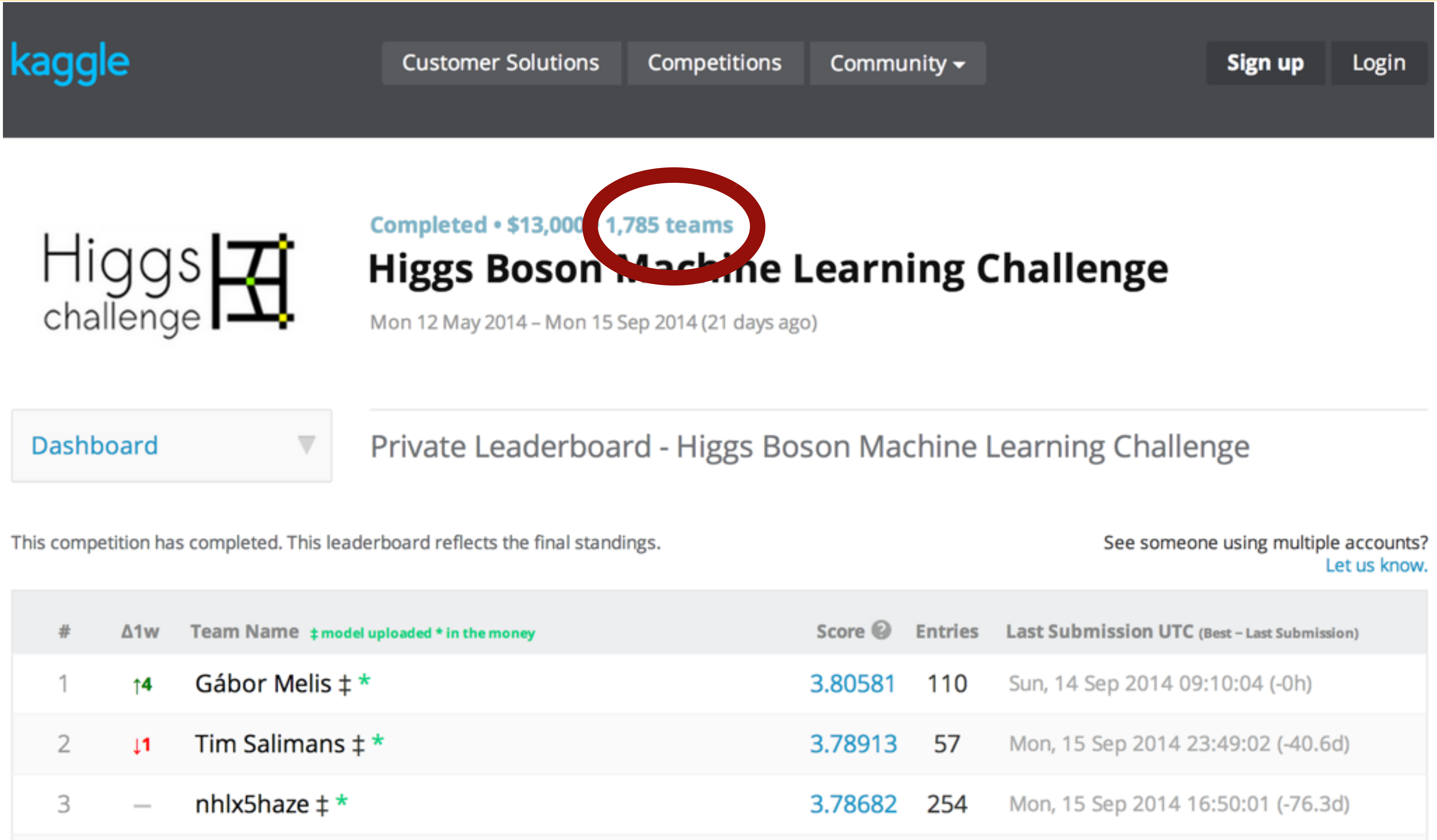


Completed • $13,000 • 1,785 teams

Higgs Boson Machine Learning Challenge

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

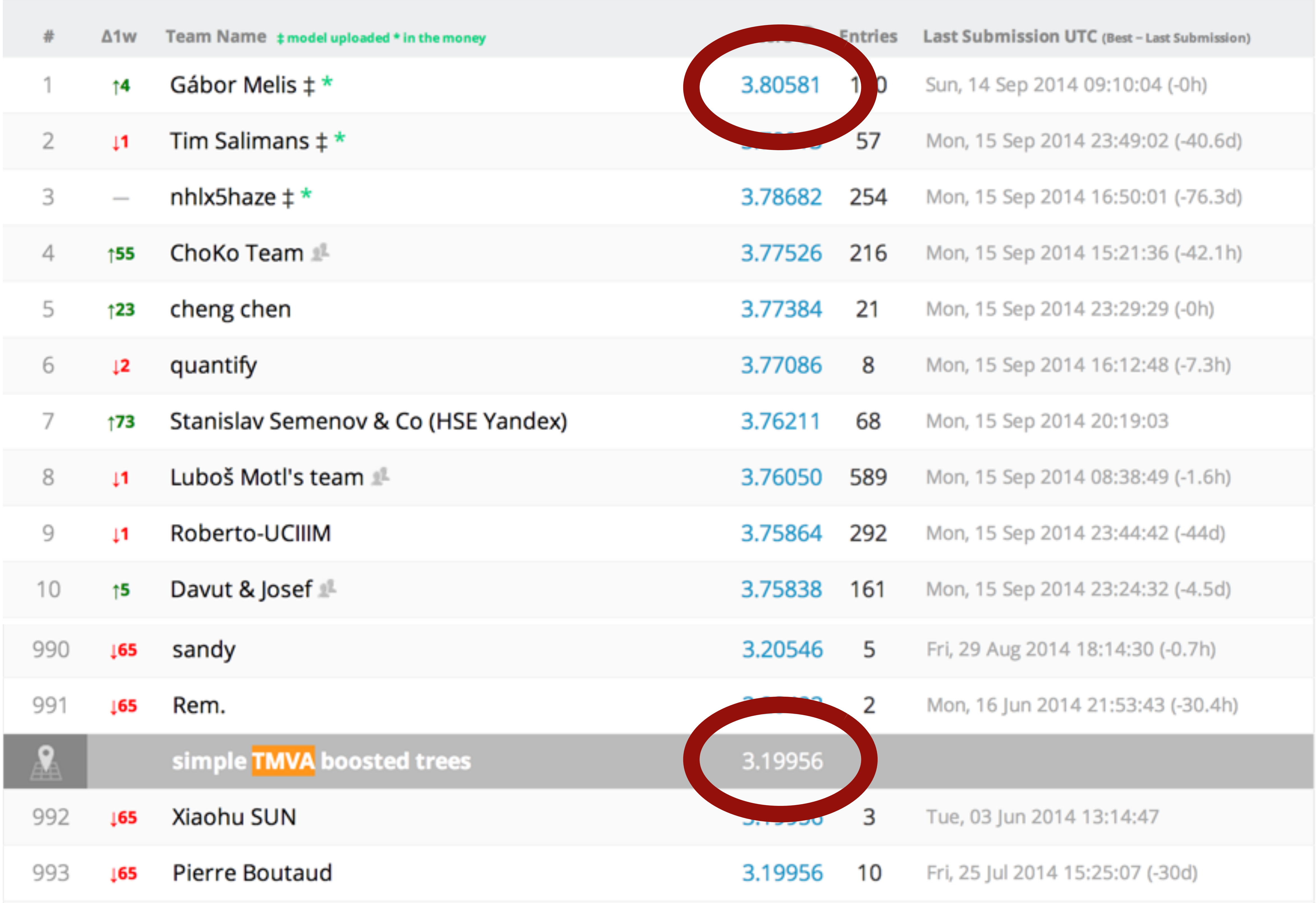
Private Leaderboard - Higgs Boson Machine Learning Challenge

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	Entries	Last Submission UTC (Best – Last Submission)
1	↑4	Gábor Melis ‡ *	3.80581	110	Sun, 14 Sep 2014 09:10:04 (-0h)
2	↓1	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)

Classification for discovery



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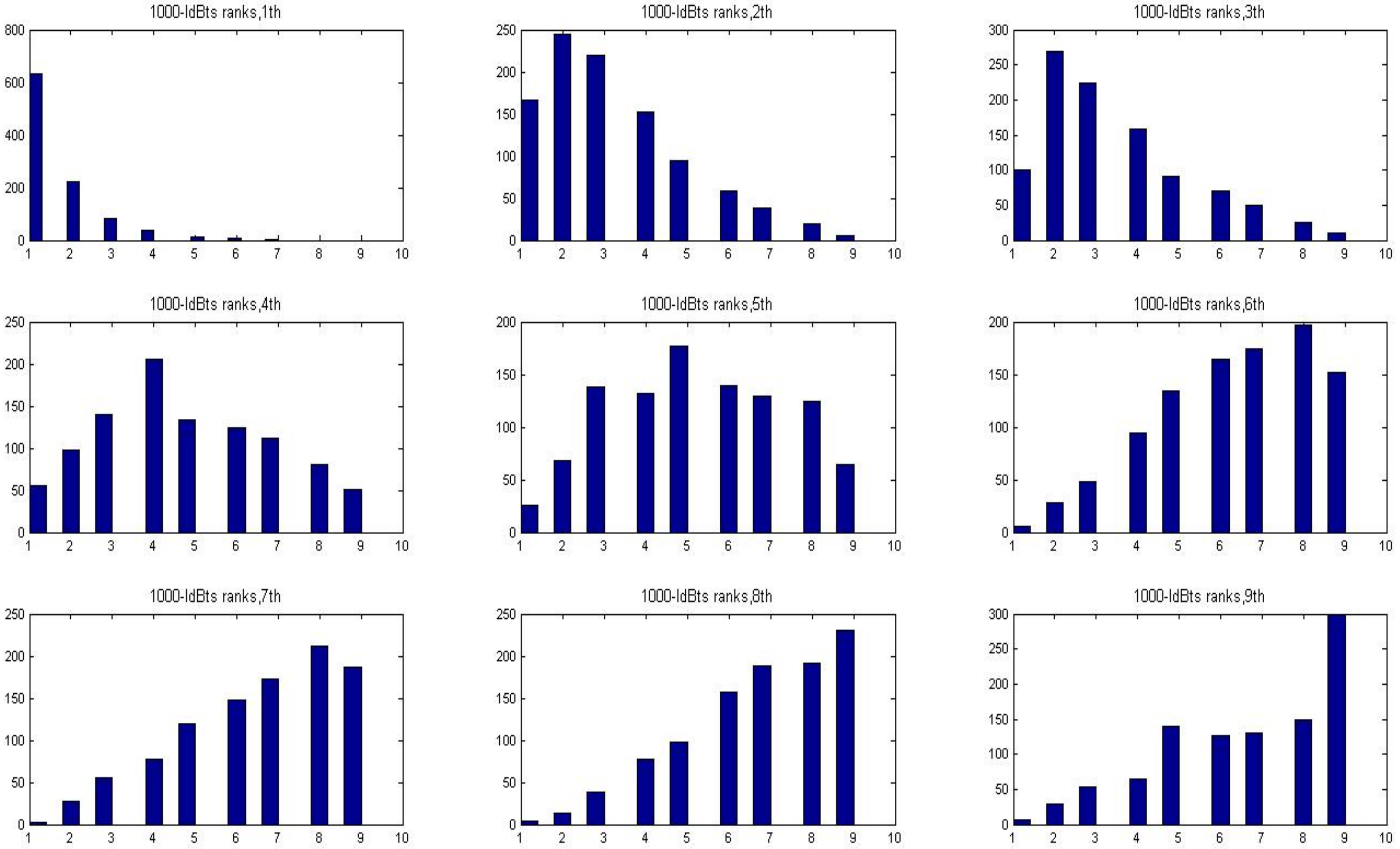
1	↑4	Gábor Melis ‡ *	3.80581	[illegible]	Sun, 14 Sep 2014 09:10:04 (-0h)
2	↓1	Tim Salimans ‡ *	[illegible]	57	Mon, 15 Sep 2014 23:49:02 (-40.6d)
3	—	nhlx5haze ‡ *	3.78682	254	Mon, 15 Sep 2014 16:50:01 (-76.3d)
4	↑55	ChoKo Team	3.77526	216	Mon, 15 Sep 2014 15:21:36 (-42.1h)
5	↑23	cheng chen	3.77384	21	Mon, 15 Sep 2014 23:29:29 (-0h)
6	↓2	quantify	3.77086	8	Mon, 15 Sep 2014 16:12:48 (-7.3h)
7	↑73	Stanislav Semenov & Co (HSE Yandex)	3.76211	68	Mon, 15 Sep 2014 20:19:03
8	↓1	Luboš Motl's team	3.76050	589	Mon, 15 Sep 2014 08:38:49 (-1.6h)
9	↓1	Roberto-UCIIIM	3.75864	292	Mon, 15 Sep 2014 23:44:42 (-44d)
10	↑5	Davut & Josef	3.75838	161	Mon, 15 Sep 2014 23:24:32 (-4.5d)
990	↓65	sandy	3.20546	5	Fri, 29 Aug 2014 18:14:30 (-0.7h)
991	↓65	Rem.	[illegible]	2	Mon, 16 Jun 2014 21:53:43 (-30.4h)
		simple TMVA boosted trees	3.19956		
992	↓65	Xiaohu SUN	3.19956	3	Tue, 03 Jun 2014 13:14:47
993	↓65	Pierre Boutaud	3.19956	10	Fri, 25 Jul 2014 15:25:07 (-30d)

ARE THE WINNING SCORES SIGNIFICANTLY DIFFERENT?



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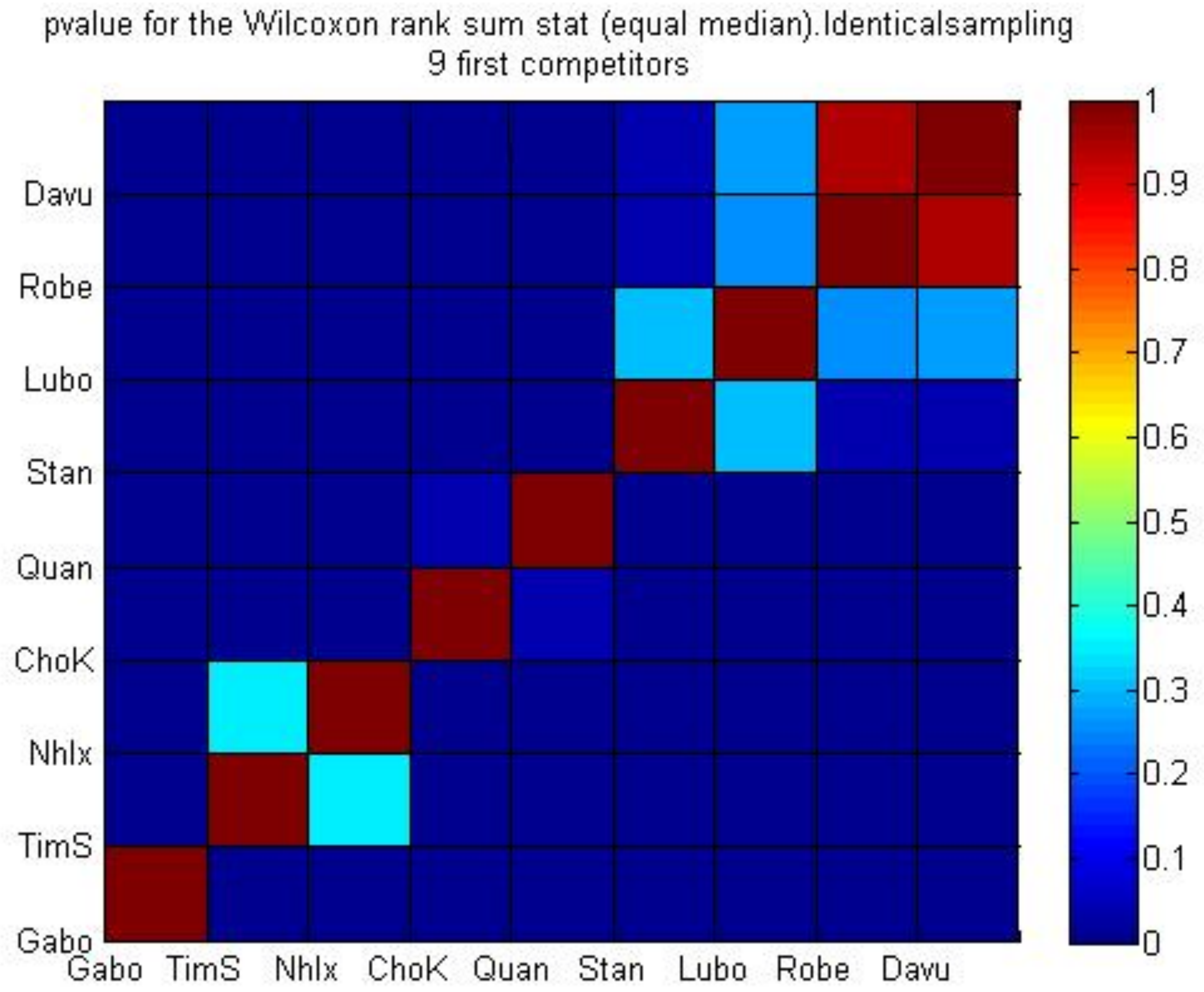
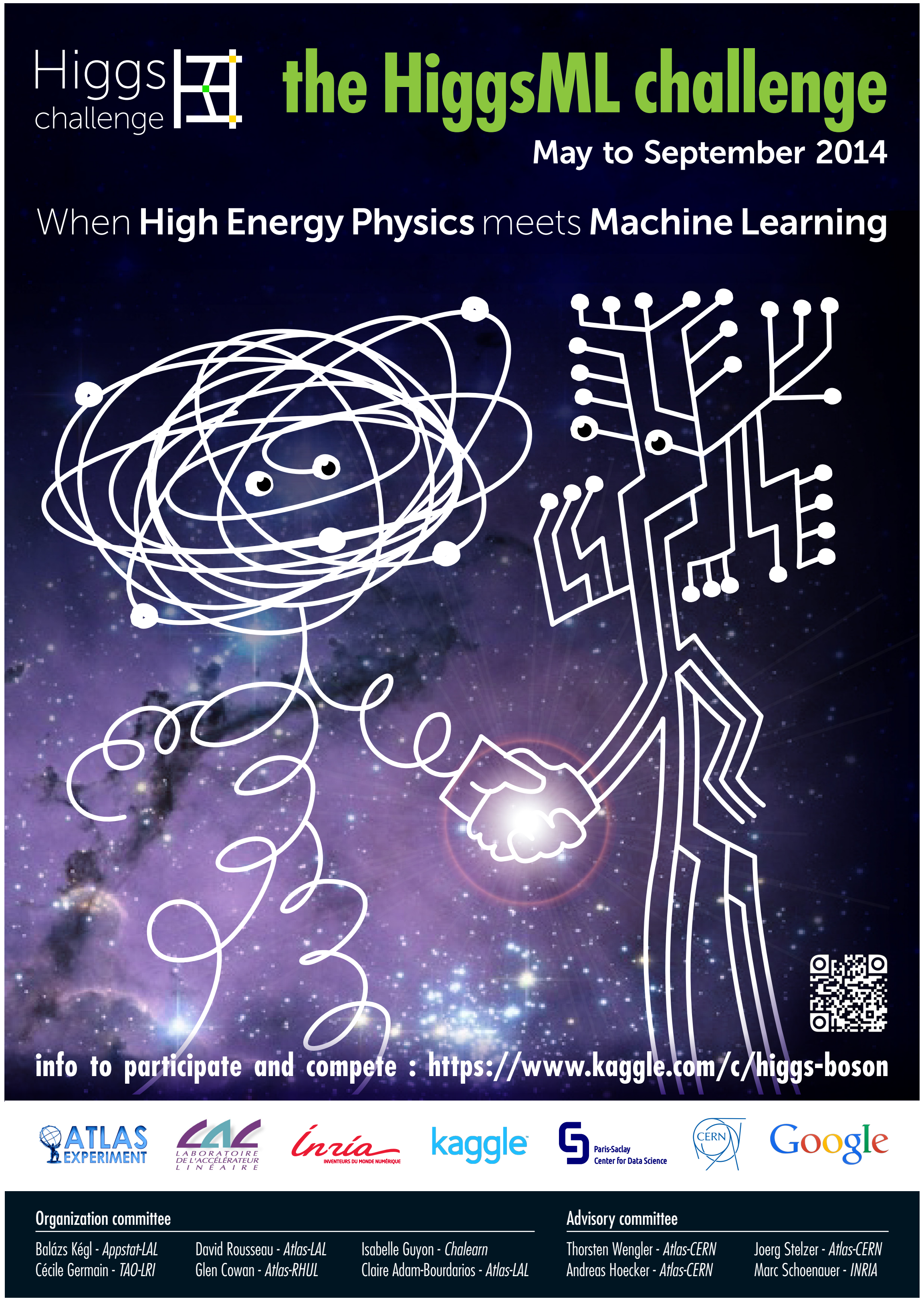


Classification for discovery

- 18 months to organize it

- 4 months to run it

- ?? months to transfer to HEP what we learned



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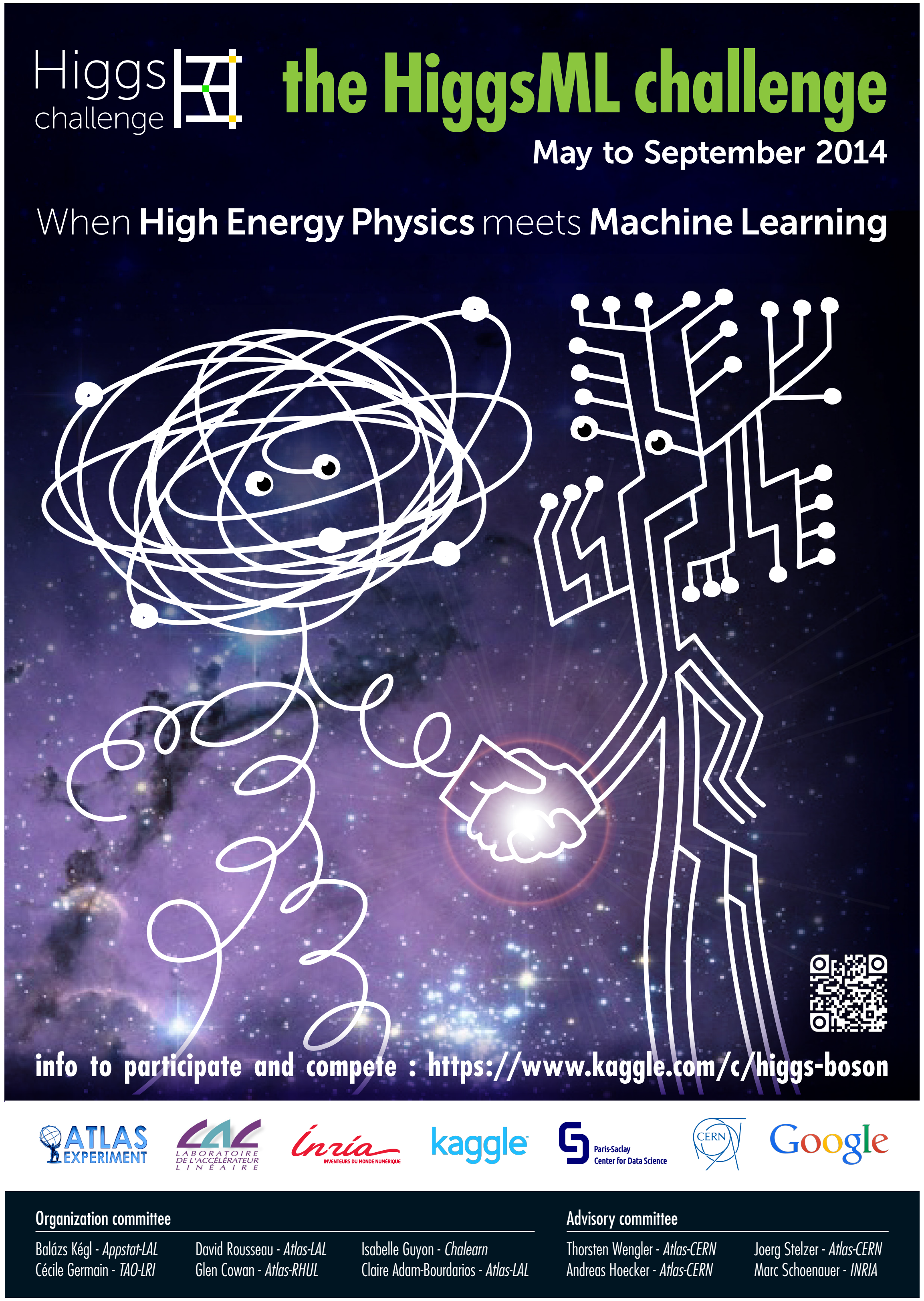
What have we learned so far?

- **Neural nets** (dropout, RLU, etc.) rule (although no slam dunk)
- **Ensemble methods** (random forest, boosting) rule
- **Meta-ensembles** of diverse models rule
- 800K points is small for this task: **careful cross-validation** rules



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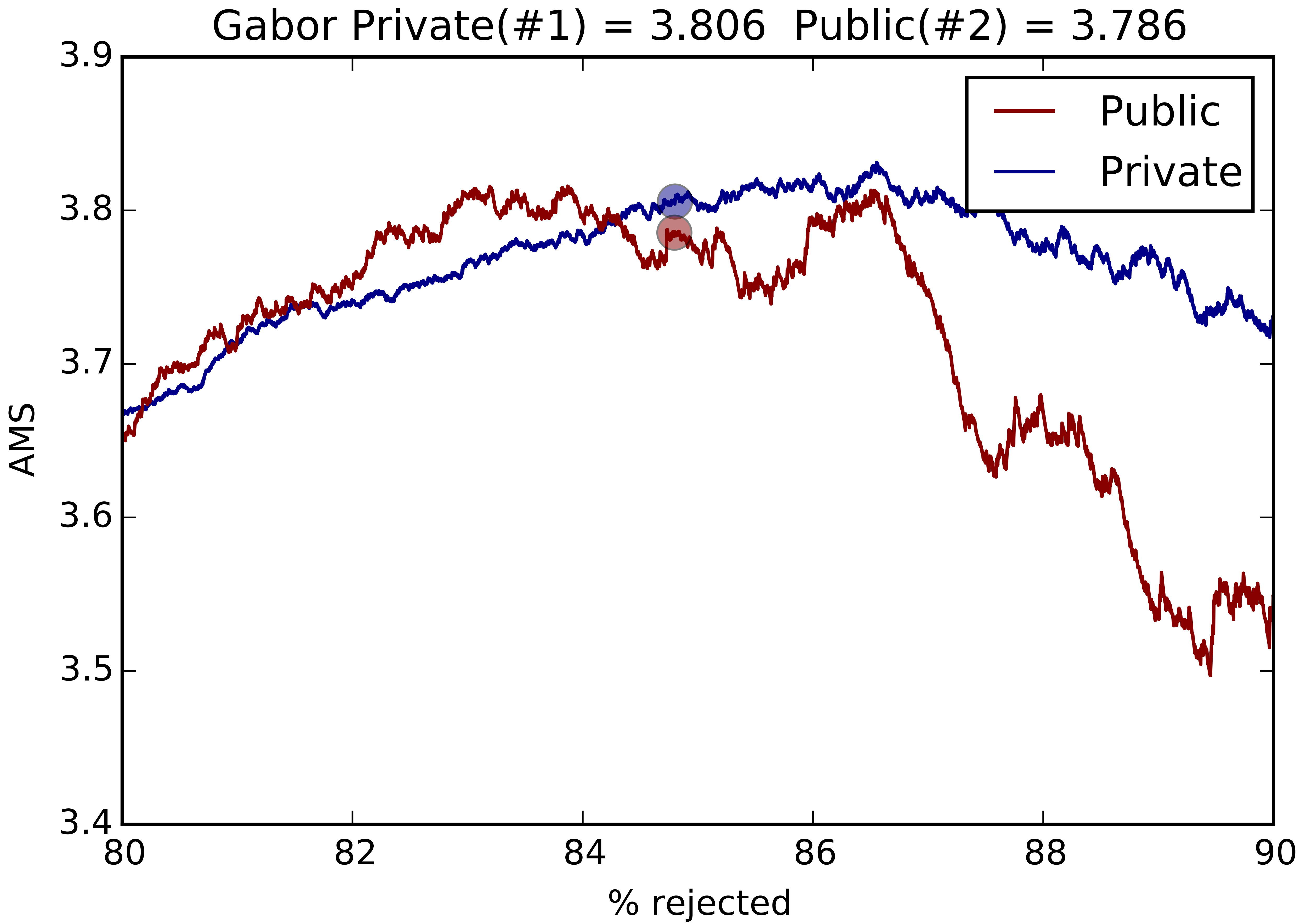
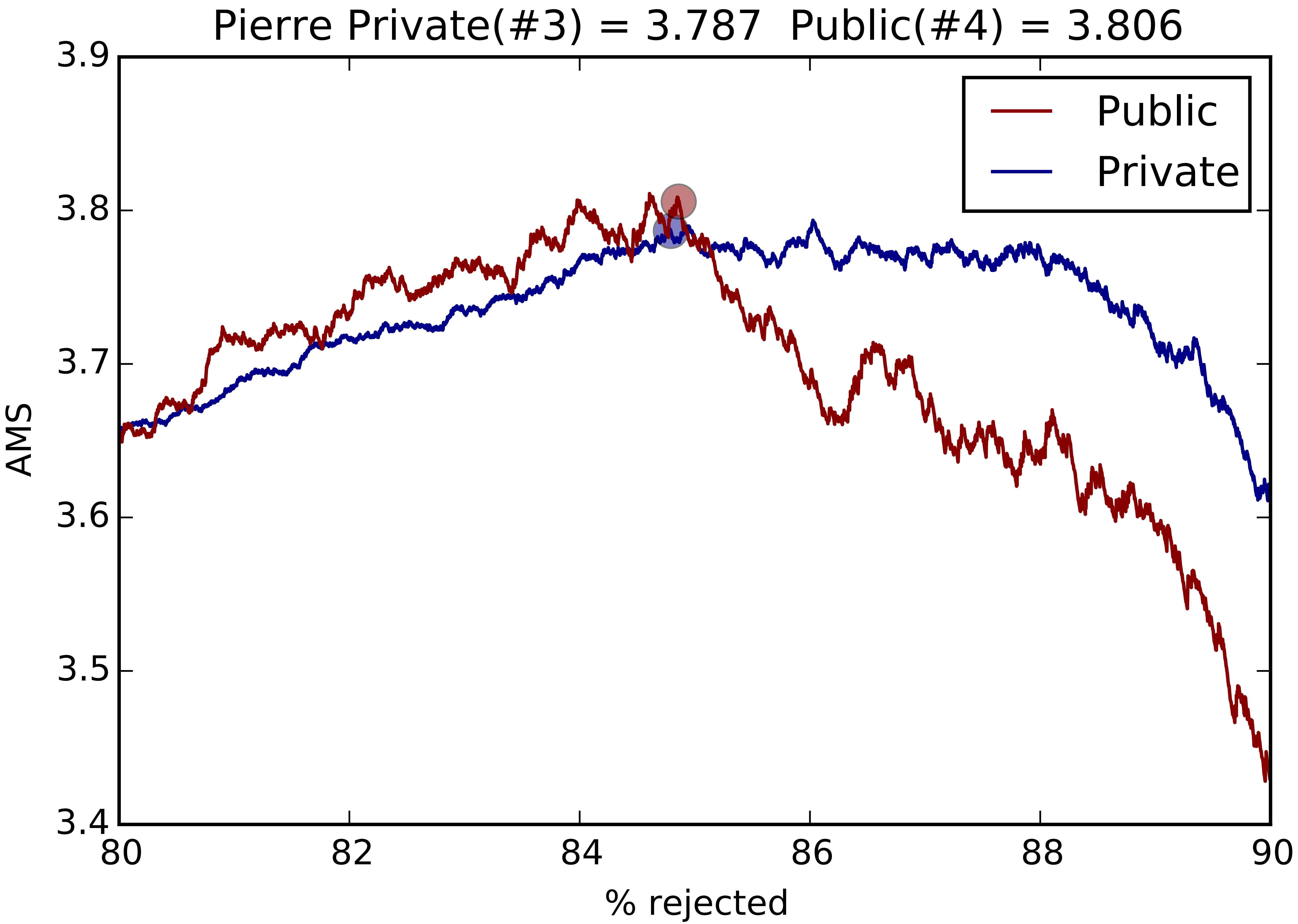
800K IS A SMALL?

- We asked participants to find good classifiers (in "smooth" AUC sense) but also to **come up with the best selection threshold**
- Optimal region contains about ~15% of the points
- Standard deviation of AMS (given the classifier and the threshold) is about **0.04** (0.08 on the public leaderboard)

800K IS A SMALL?

Find the maximum of a noisy diffusion-like process


Gabor Private(#1) = 3.806 Public(#2) = 3.786
AMS
3.9
3.8
3.7
3.6
3.5
3.4
80
82
84
86
88
90
% rejected
Public
Private


Pierre Private(#3) = 3.787 Public(#4) = 3.806
Public
Private
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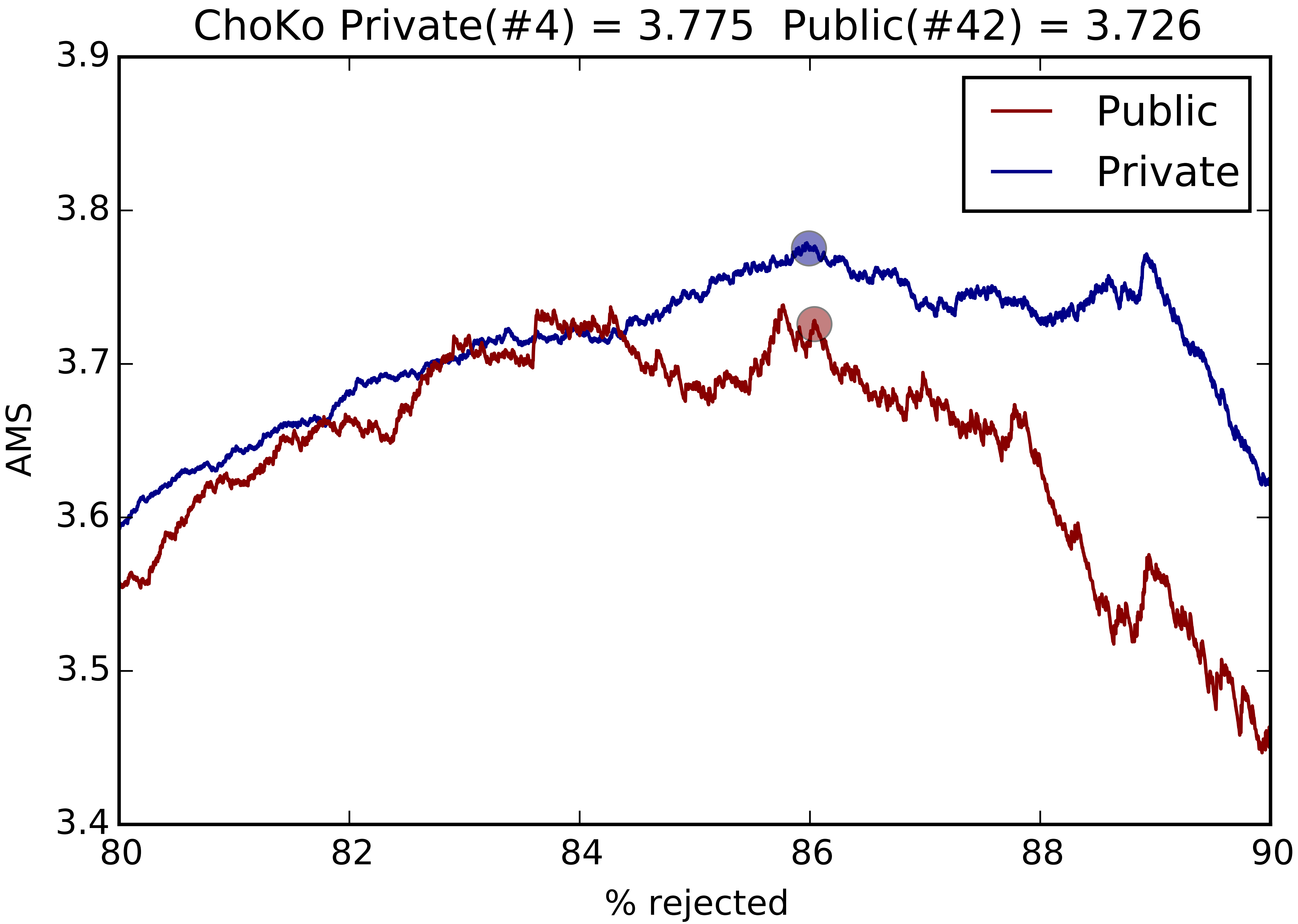
ChoKo Private(#4) = 3.775 Public(#42) = 3.726
AMS
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3.7
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% rejected
80
82
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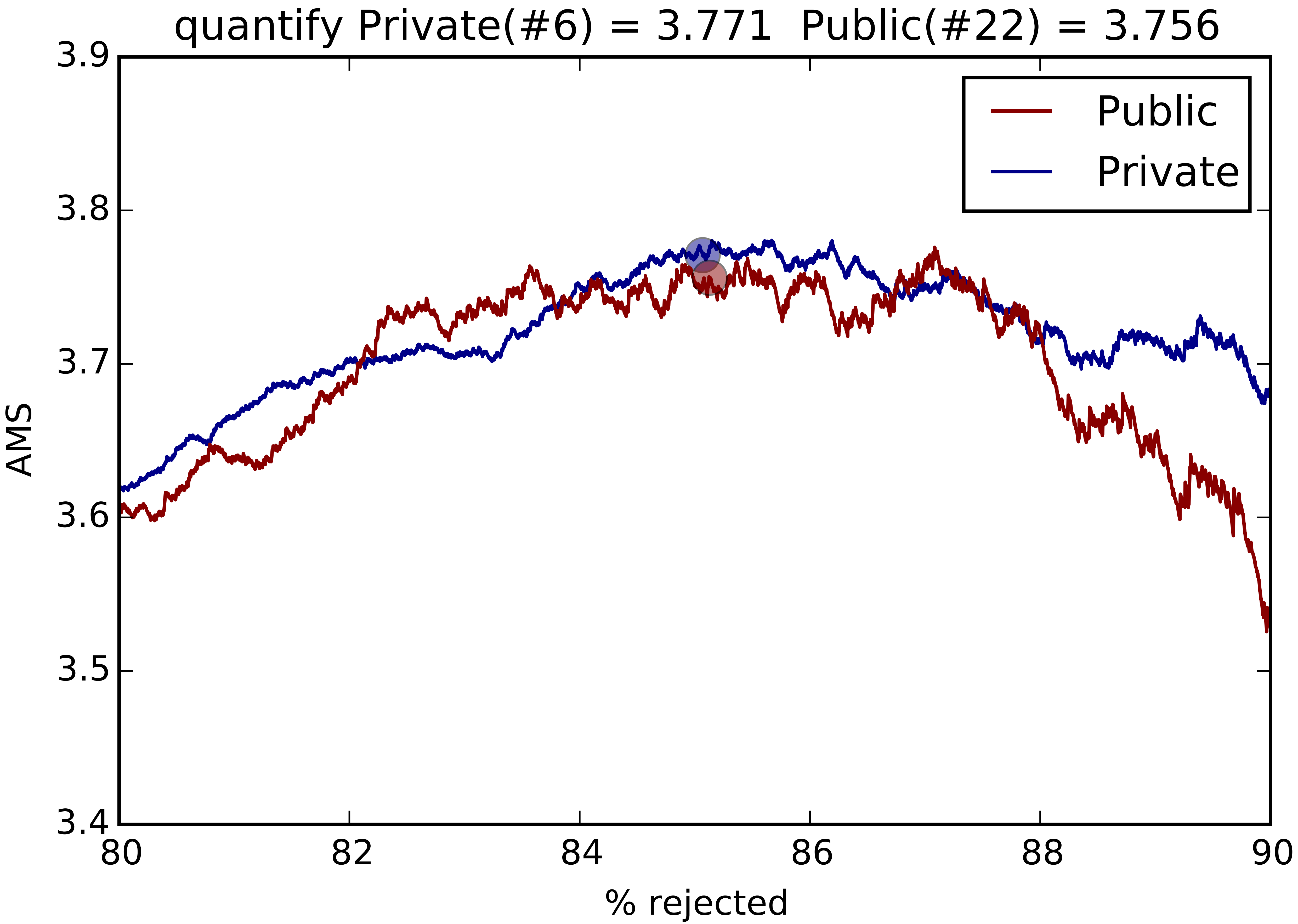
quantify Private(#6) = 3.771 Public(#22) = 3.756
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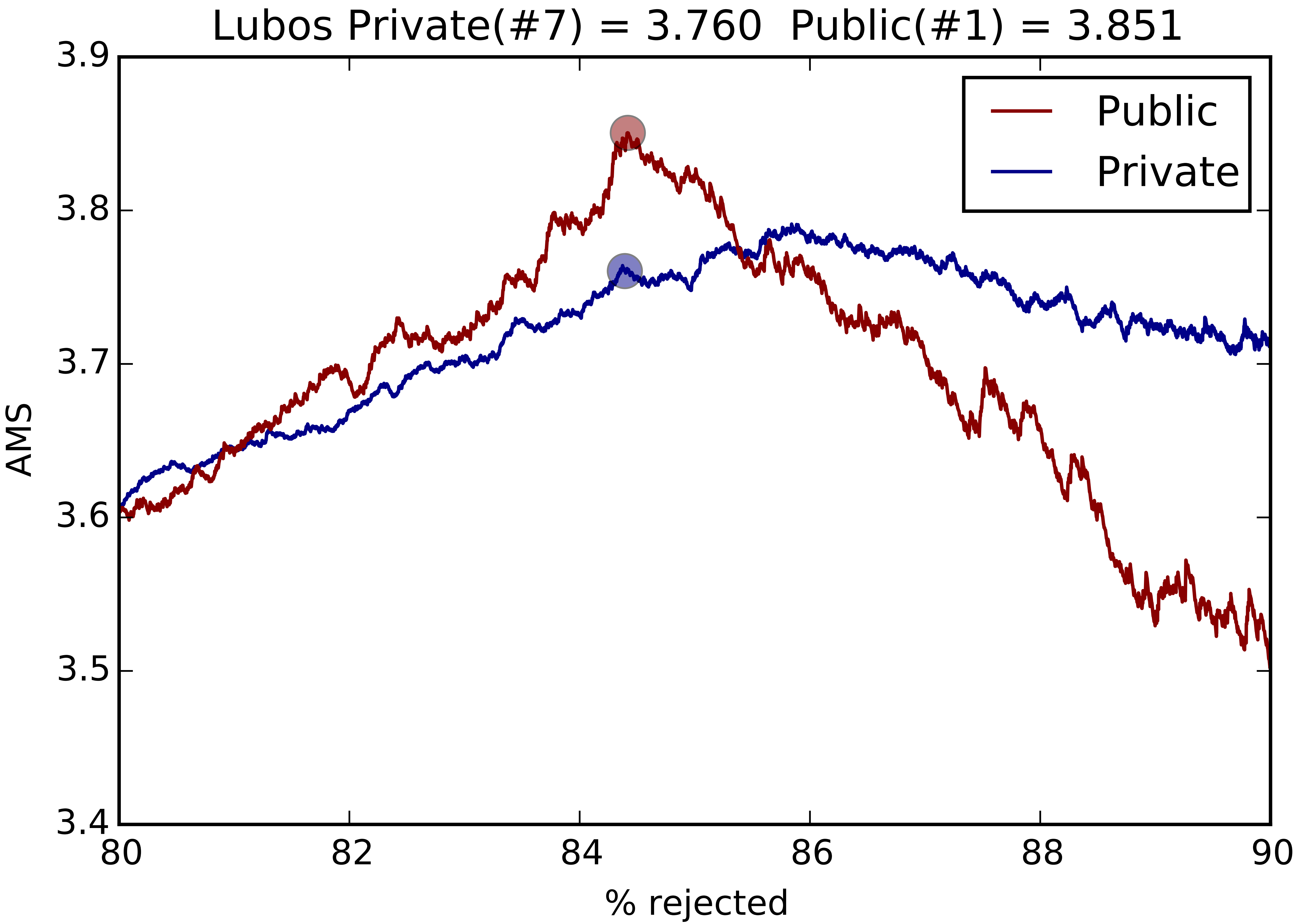
Lubos Private(#7) = 3.760 Public(#1) = 3.851
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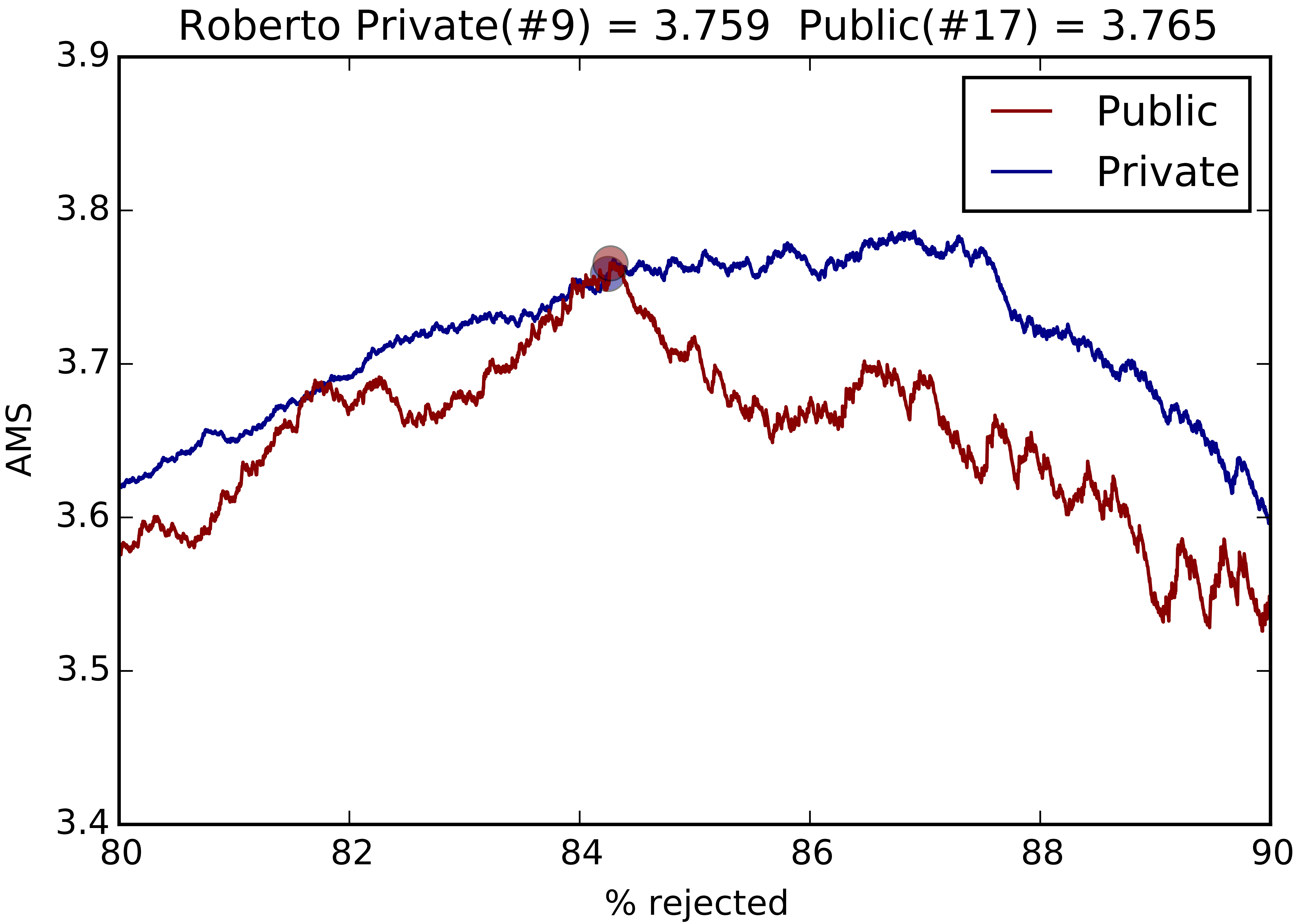
Roberto Private(#9) = 3.759 Public(#17) = 3.765
Public
Private
AMS
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3.5
3.4
80
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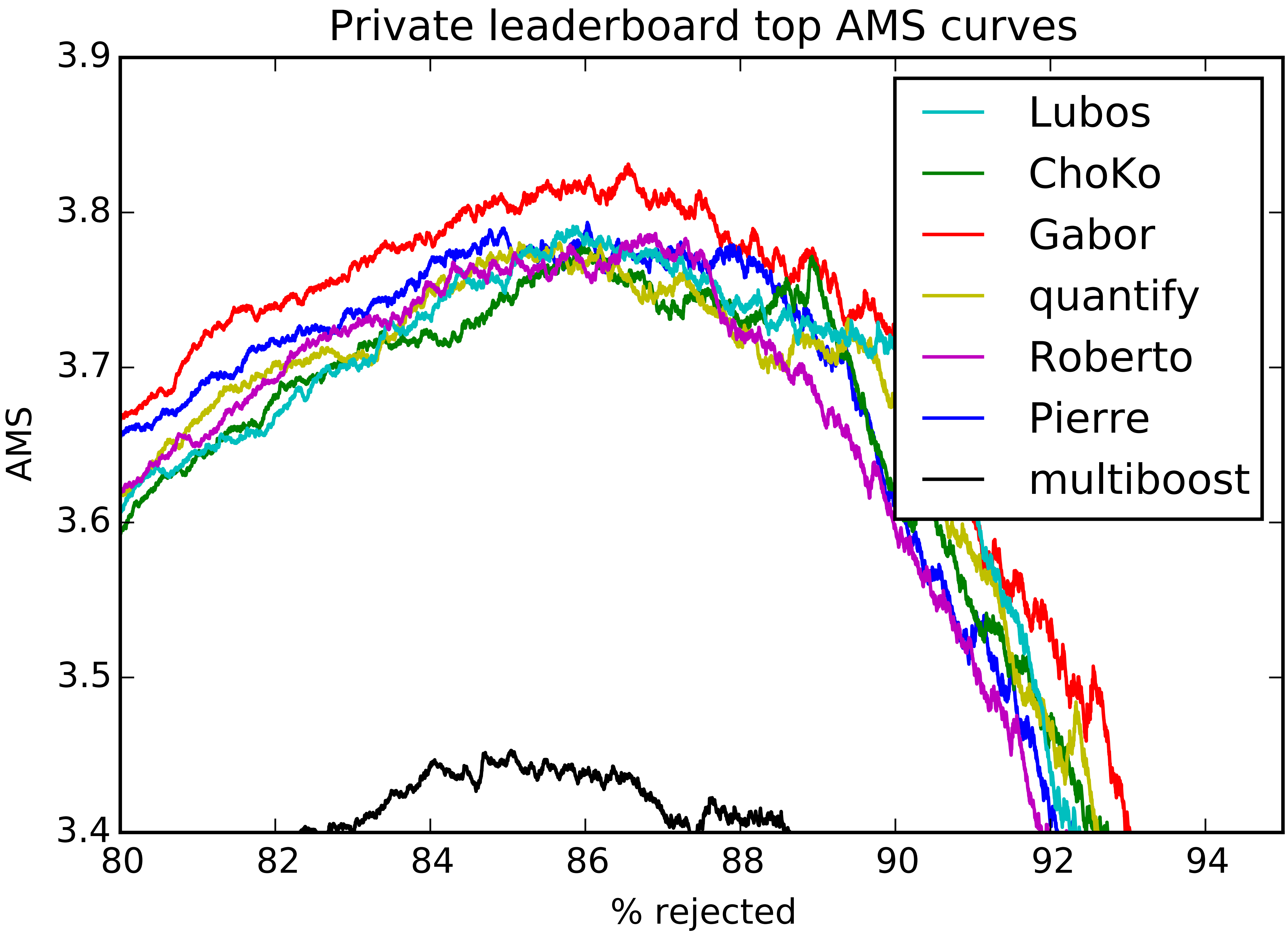
% rejected



Private leaderboard top AMS curves
AMS
% rejected
3.4
3.5
3.6
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3.8
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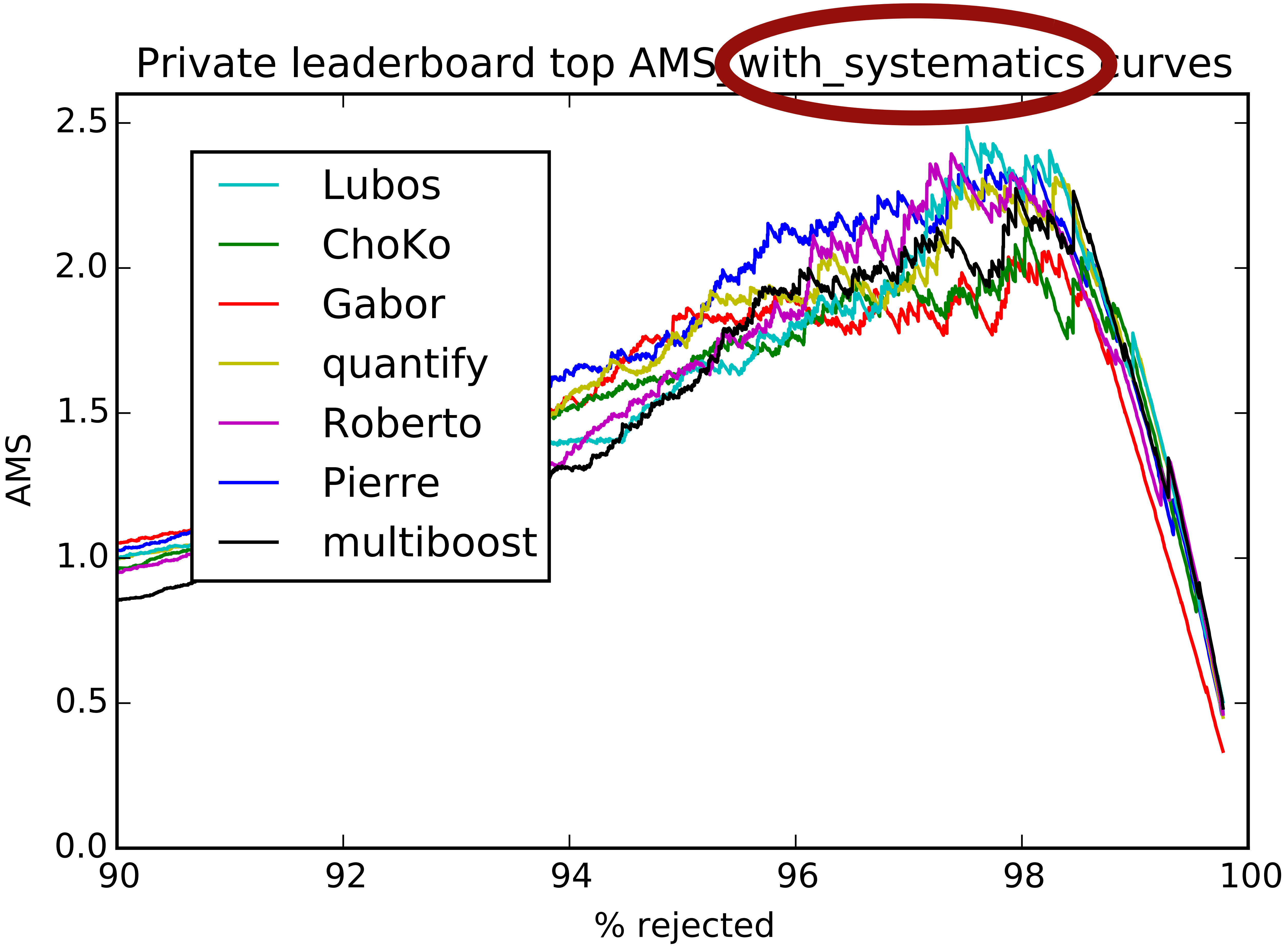
94
Lubos
ChoKo
Gabor
quantify
Roberto
Pierre
multiboost


Private leaderboard top AMS_with_systematics curves
Lubos
ChoKo
Gabor
quantify
Roberto
Pierre
multiboost
AMS
0.0
0.5
1.0
1.5
2.0
2.5
90
92
94
96
98
100
% rejected

META

- A data challenge is a great way to
  - generate visibility
  - human resources
  - optimize a tiny segment of the complete workflow
- Limitations
  - technical constraints (e.g., no server-side execution)
  - sociological constraints (should not be too far from an off-the-shelf problem)
  - emphasizes competition instead of collaboration

Data will be available soon

http://opendata.cern.ch/education/ATLAS

ML IN HIGH-ENERGY PHYSICS

- Budgeted classification for online triggers
- Maximizing the discovery significance and other exotic metrics
- Deep learning for getting closer to raw data
- How to be robust to systematic errors

HEPML workshop at NIPS14

Saturday 13 December 2014

Session 1 - Level 5, room 511 c (08:30-10:00)

time	title	presenter
08:30	Welcome (00h15')	KÉGL, Balázs
08:45	HEP&ML and the HiggsML challenge (00h35')	KÉGL, Balázs
09:20	Embedding ML in Classical Statistical tests used in HEP (invited talk) (00h40')	CRANMER, Kyle

Coffee break - Level 5, room 511 c (10:00-10:30)

Session 2 - Level 5, room 511 c (10:30-12:10)

time	title	presenter
10:30	Presentation of the winner of the HiggsML challenge (00h20')	MELIS, Gábor
10:50	Presentation of the runner up of the HiggsML challenge (00h20')	SALIMANS, Tim
11:10	Presentation of the winner of the HEP meets ML prize (00h20')	CHEN, Tianqi
11:30	Real time data analysis at the LHC : present and future (00h40')	GLIGOROV, Vava

Session 3 - Level 5, room 511 c (15:00-16:30)

time	title	presenter
15:00	Machine Learning for Ultra-High-Energy Physics (invited talk) (00h40')	WHITESON, Daniel
15:40	Weighted Classification Cascades for Optimizing Discovery Significance in the HiggsML Challenge (00h20')	MACKEY, Lester
16:00	Consistent optimization of AMS by logistic loss minimization (00h20')	KOTLOWSKI, Wojciech

Coffee break - Level 5, room 511 c (16:30-17:00)

Session 4 - Level 5, room 511 c (17:00-18:30)

time	title	presenter
17:00	Ensemble of maximied Weighted AUC models for the maximization of the median discovery significance (00h20')	MORALES, Roberto Diaz
17:20	Deep Learning In High-Energy Physics (invited talk) (00h40')	BALDI, Pierre
18:00	Panel discussion (00h30')	