Based on arXiv:2405.12972

[Github] [Google Colab]

Sophon meets LHC:
Accelerating resonance discovery via signature-oriented pre-training

Congqiao Li (李聪乔), ***Peking University***

based on the work with our colleagues in the CMS Collaboration:

Antonios Agapitos[1], Jovin Drews[2], Javier Duarte[3], Dawei Fu[1], Leyun Gao[1], Raghav Kansal[3], Gregor Kasieczka[2], Louis Moureaux[2], Huilin Qu[4], Cristina Mantilla Suarez[5], Qiang Li[1]

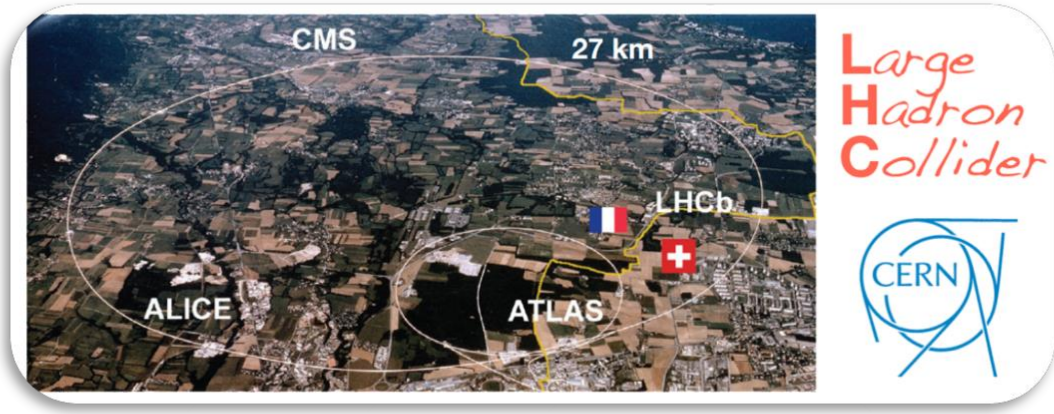
1) Peking U. 2) Hamburg U. 3) UC San Diego 4) CERN 5) FNAL

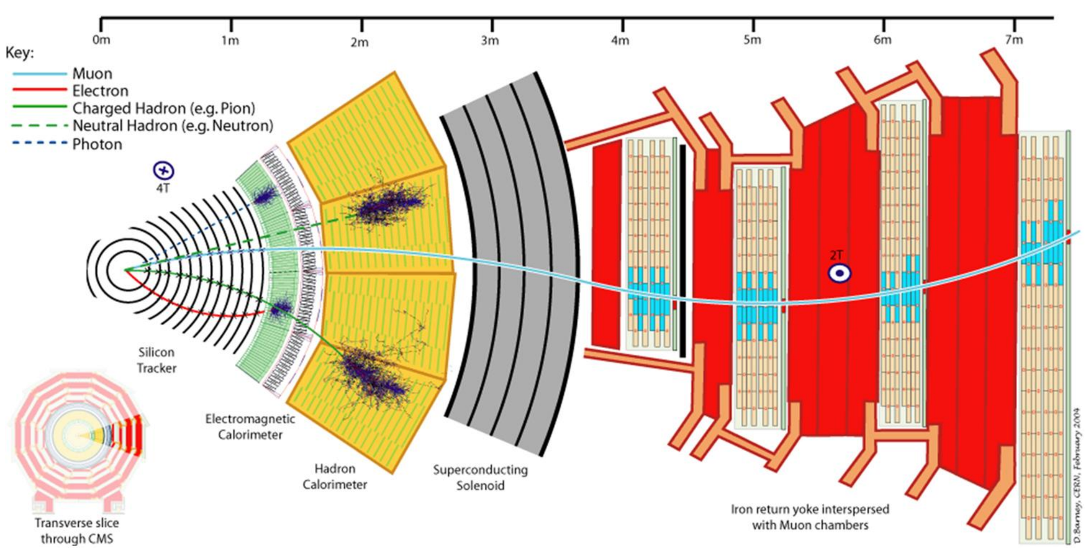
also thanks **Yuzhe Zhao[1]** *for his contribution*

Quantum Computing and Machine Learning Workshop 2024, Changchun

6 August, 2024

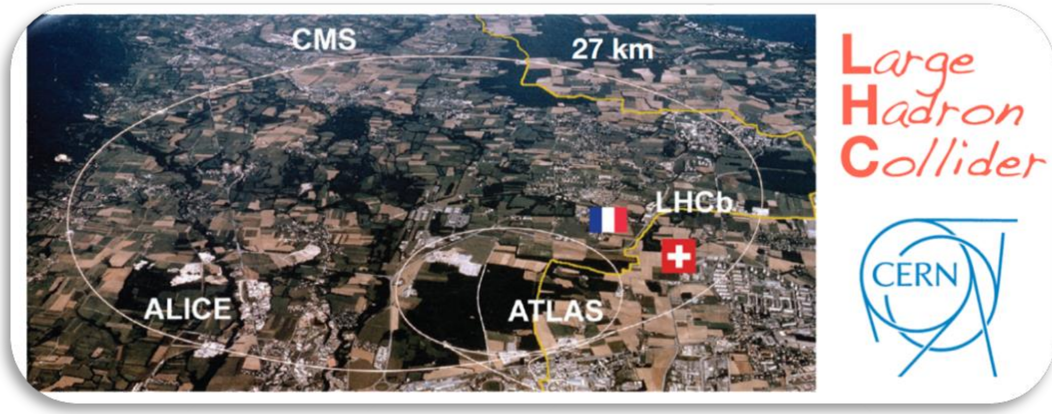
LHC physics × the era of deep learning

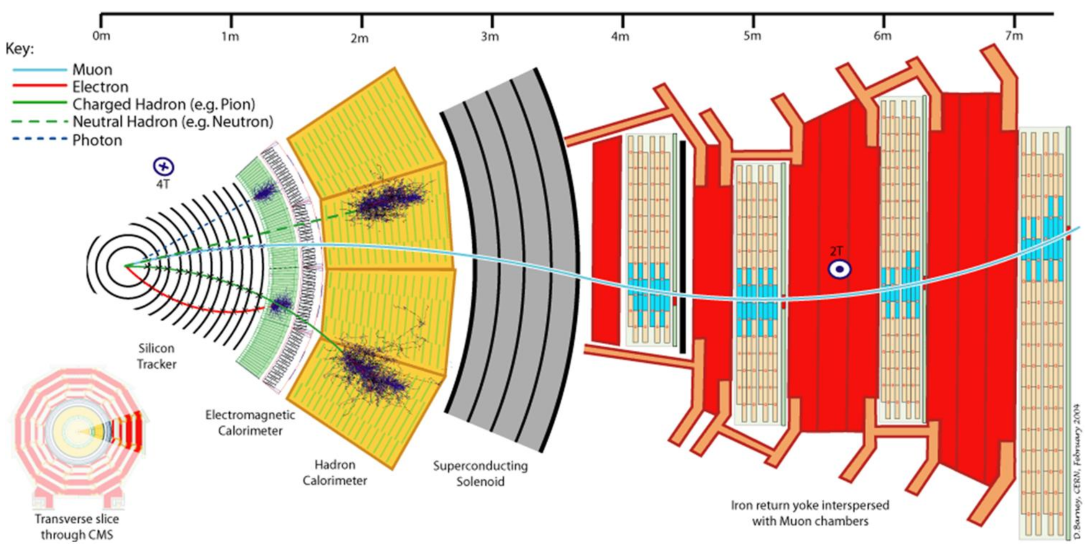




- ➔ The LHC: current world's largest particle collider
- ➔ Physics programs on LHC: reveal the fundamental theory of matters
- ➔ ATLAS and CMS: general-purpose detectors for precise SM measurement and **searching of BSM**

LHC physics × the era of deep learning





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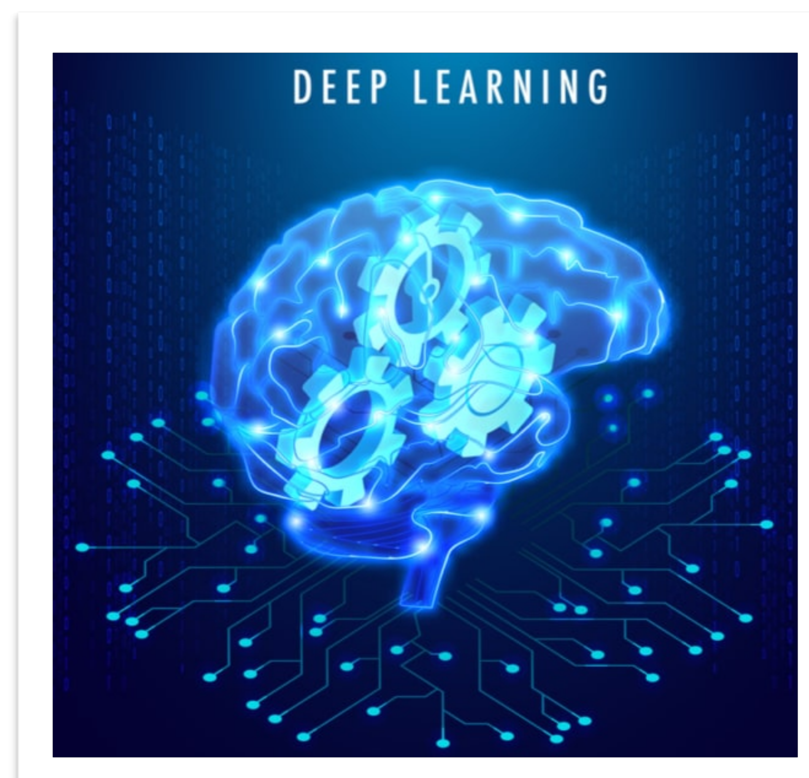
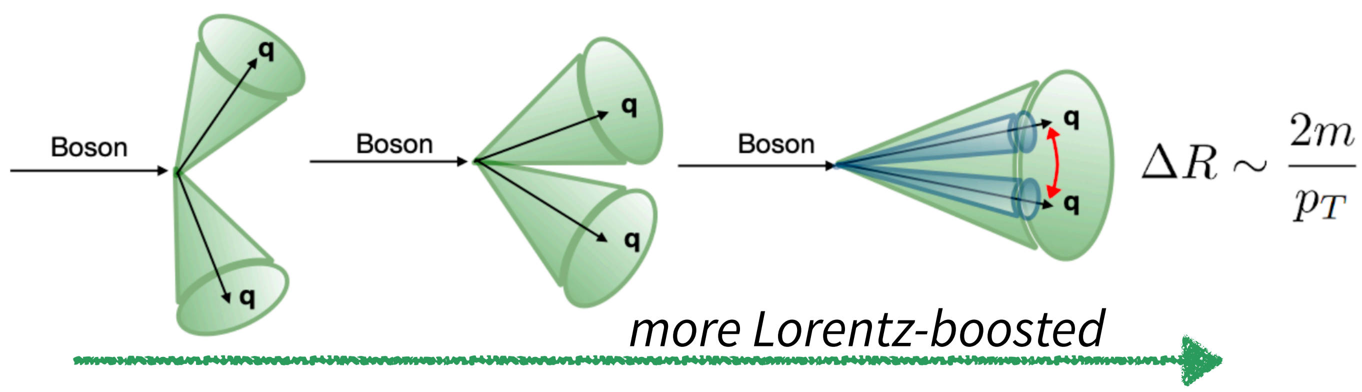
- ➔ ATLAS and CMS: general-purpose detectors for precise SM measurement and **searching of BSM**

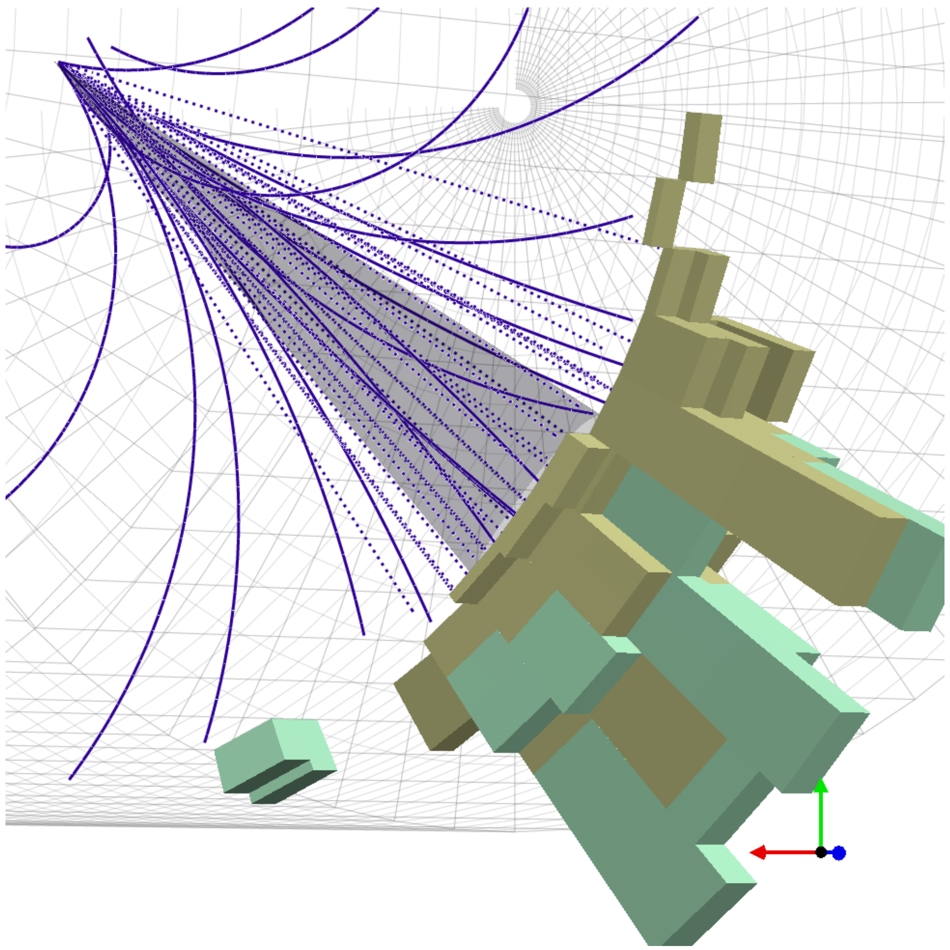
- ✤ *Deep learning (AI) is brining a technological leap in analyzing LHC data*
- ✤ *It is intriguing to think where the future possibility lies*



Boosted topology – a booster to sensitivity for LHC physics

➔ Large-*R* jets: an important handle to analyze boosted topologies at the LHC





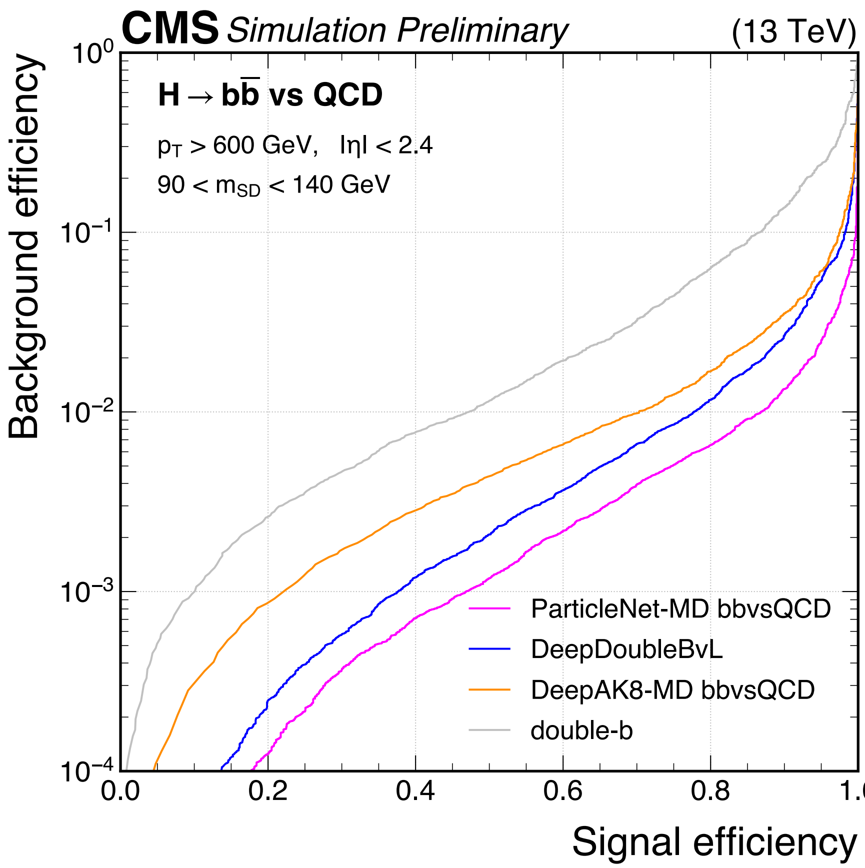
- Applications to Higgs/di-Higgs/BSM searches in boosted **H(X)→b$\bar{b}$/c$\bar{c}$** final states have been a success

➔ *Suitable for deploying cutting-edge deep learning techniques*

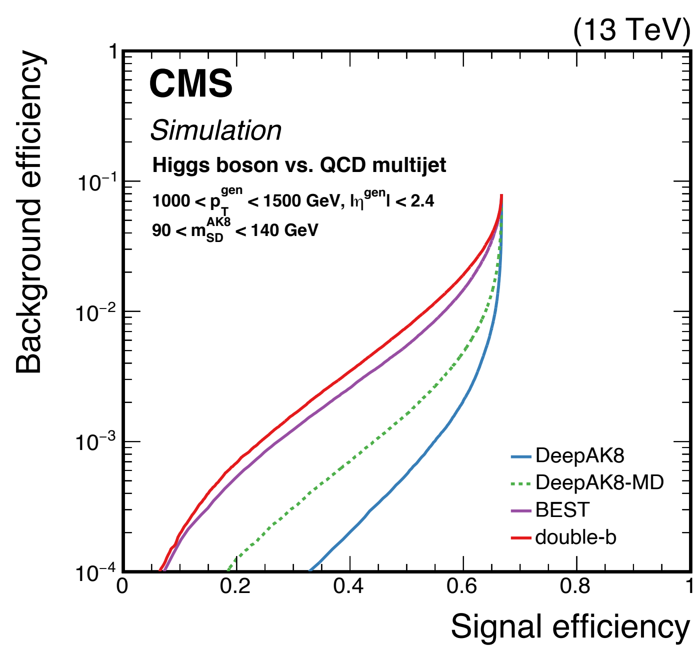
- most complex object to handle at the LHC (up to ~100 constituent particles)
- advanced DNNs greatly boost analysis sensitivity

Inspiring progress on H→b$\bar{b}$/c$\bar{c}$ tagging

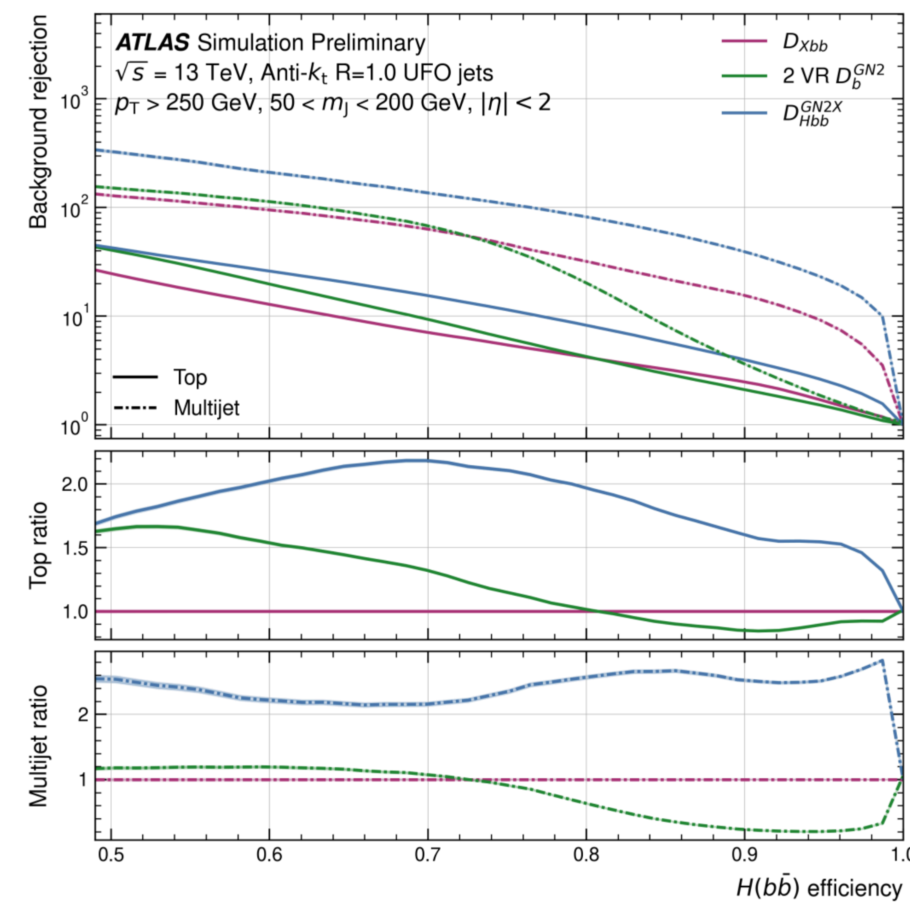
CMS-PAS-BTV-22-001



JINST 15 (2020) P06005



ATL-PHYS-PUB-2023-021



An upgrade of network

DeepAK8 → ParticleNet:

x5 📈 QCD background rejection

Note: back to the results 5 years ago

DeepAK8 tagger already has **~x5** 📈 improved background rejection than early methods

Recent GN2X tagger:

~x3 📈 QCD and x2 top background rejection

Inspiring progress on H→$b\bar{b}$/$c\bar{c}$ tagging

Implications

Advancements in NN design are the true driving force behind the gains in sensitivity!

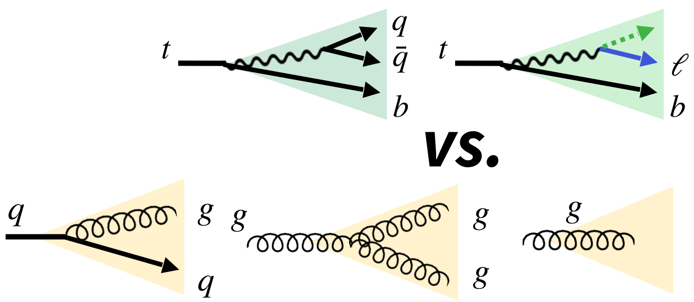
- **However, this tool is available only in limited phase space**
  (e.g. H→bb, W→qq, t→bqq…)

- **Can we extend its usage to all possible boosted phase spaces?**
- **If we can boost the sensitivity by *x10* in many phase spaces, will it accelerate the "next potential discovery" of a new resonance?**

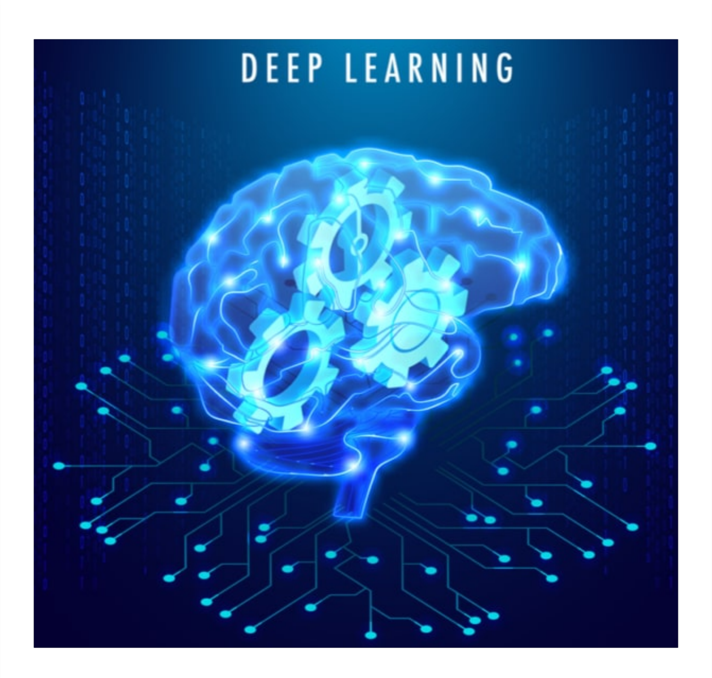
Propose “Large model for large-scale classification”

View from jet tagging

- ➔ Instead of training dedicated jet taggers, we consider **multi-class classification** with N(class) reaches $o(100)$
  - ❖ statistical insights: an ideal multi-class classifier is a stack of ideal binary classifiers (next slide)
- ➔ The model should be **large** → carry enough capacity
- ➔ The classes should be comprehensive → **tagging ability can be further generalized by fine-tuning**



View from a pre-training solution



- ➔ We own a comprehensive jet dataset, and we hope to pre-train **a foundational model** to facilitate **all** LHC analyses exploring the large-R jet
- ➔ Set the training task: let the model learn to connect **“what a jet is like”** to **“which truth signature the jet reveals”** (= jet label in our case)
  - ❖ “jet labels” are simple signatures to explore
    → pre-training it as a classifier is just a starting point in this sense!

Statistical property of multi-class classifier

→ Statistical theory shows that:

A **multi-class** classifier with minimum **cross-entropy loss** **estimates the probability ratios** on the input classes:

$$g_i(\mathbf{x}) = \frac{p(\text{class} = i \,|\, \mathbf{x})}{\sum_{j=1}^{N_{\text{out}}} p(\text{class} = j \,|\, \mathbf{x})}$$

hence it contains all the information the ideal $N(N-1)$ binary classifiers can do

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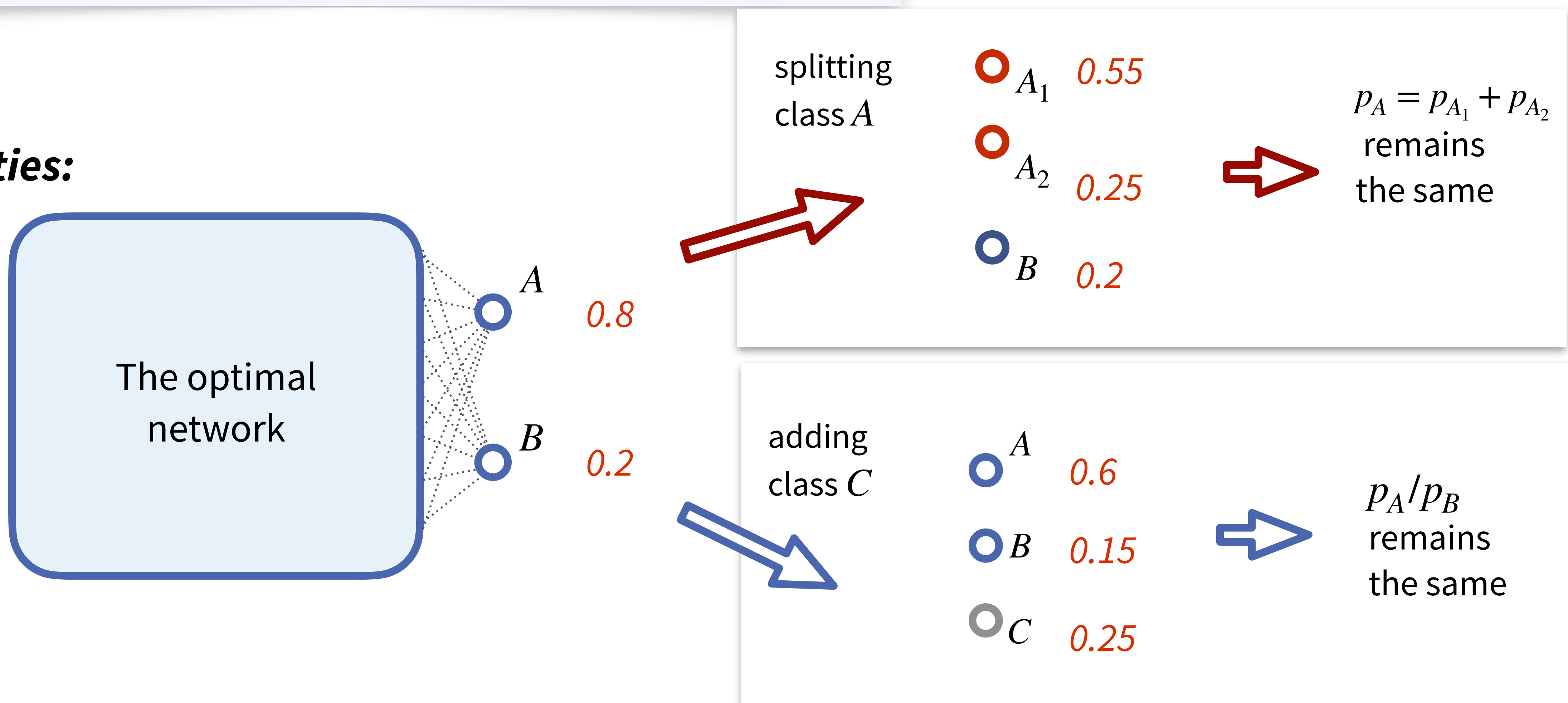
Two properties:



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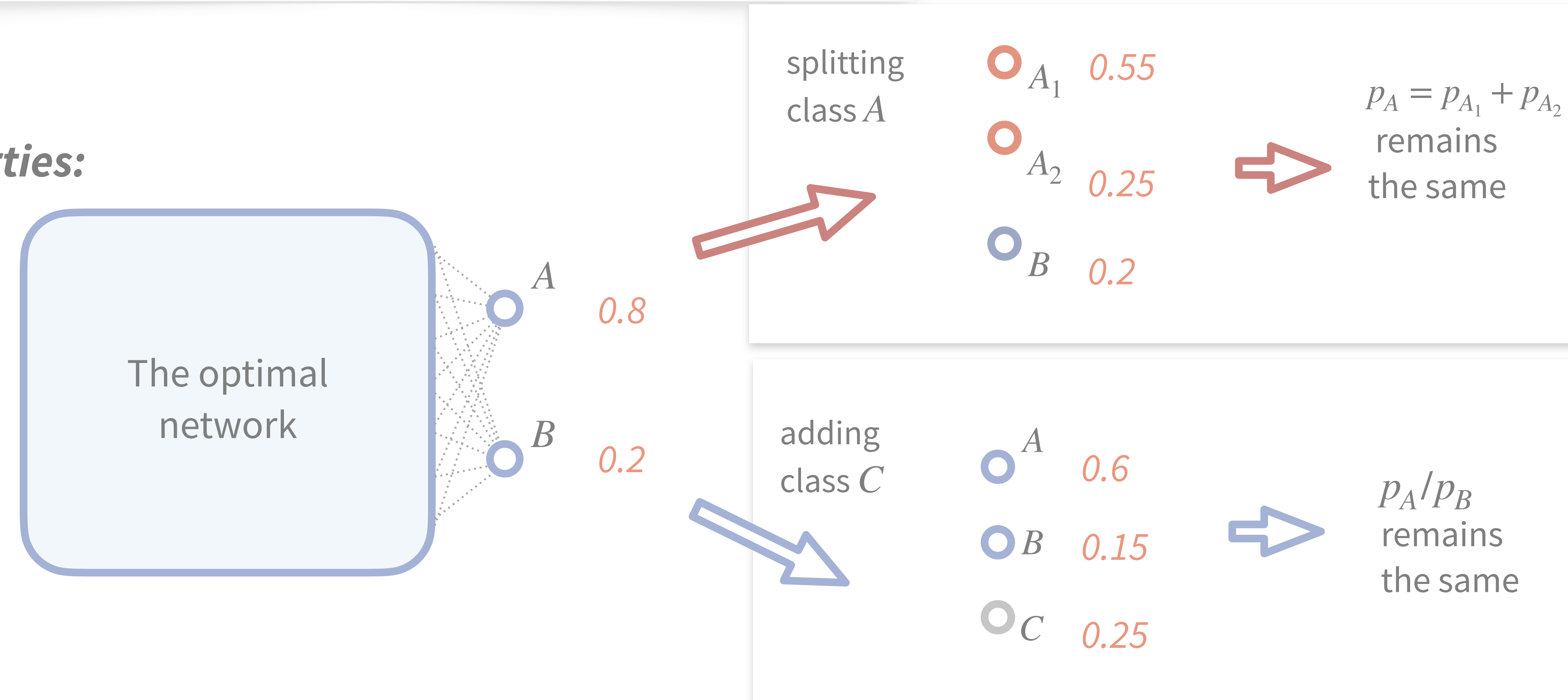
The key question in this context

Does the model's capacity still enable us to reach the best achievable performance in existing tasks?

Our result will show: Yes.

hence it contains all the information the ideal $N(N-1)$ binary classifiers can do

Two properties:



Introducing Sophon

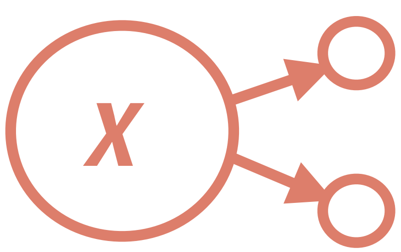
arXiv:2405.12972
https://github.com/jet-universe/sophon

➔ We explore this possibility in the CMS experiment first, and also in a recent pheno work:

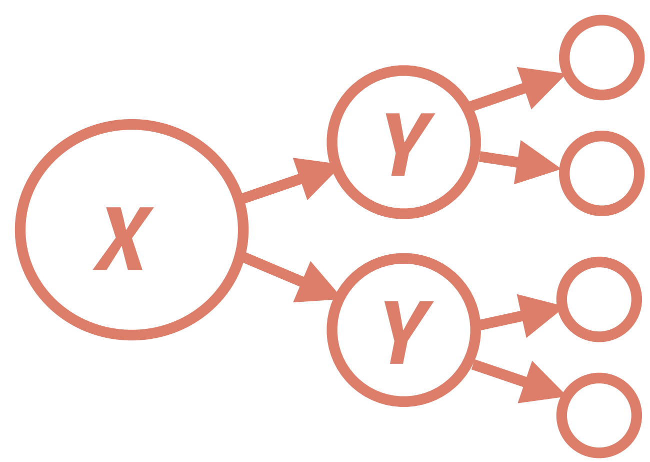
- **Signature-Oriented Pre-training for Heavy-resonant ObservatioN**
- the model is based on Particle Transformer (**ParT**) architecture
- a pre-trained model on a comprehensive dataset: **JetClass-II**
  - ***finely categorized labels:***

[H.Qu, CL, S.Qian. ICML 2022]
The current "state-of-the-art" on large-scale dataset ***(o(100M), close to experimental setup)***

Resonant jet:
X→ 2 prong

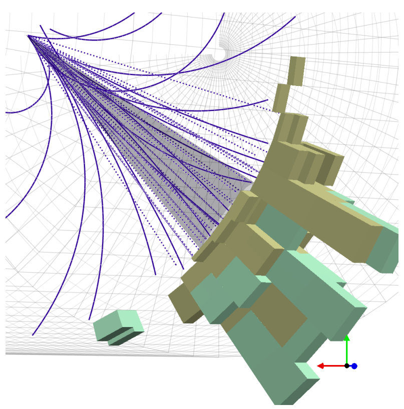


Resonant jet:
X→ 3/4 prong



bb/cc/ss/qq/gg/ee/μμ/ττ
bc/bq/cs/cq
eν/μν/τν

QCD jets



contributed final states: ***bb/cc/ss/qq/gg/ee/μμ/ττ bc/bq/cs/cq***

all combination of Y decays, resulting to 4-prong or 3-prong

Key property: we do not focus on any specific *X* and *Y* masses
Their masses are variables: ranges from 20-500 GeV

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The current "state-of-the-art" on large-scale dataset ***(o(100M), close to experimental setup)***

Major types	Index range	Label names
Resonant jets: $X \to 2$ prong	0–14	bb, cc, ss, qq, bc, cs, bq, cq, sq, gg, ee, $\mu\mu$, $\tau_h\tau_e$, $\tau_h\tau_\mu$, $\tau_h\tau_h$
Resonant jets: $X \to 3$ or 4 prong	15–160	$bbbb$, $bbcc$, $bbss$, $bbqq$, $bbgg$, $bbee$, $bb\mu\mu$, $bb\tau_h\tau_e$, $bb\tau_h\tau_\mu$, $bb\tau_h\tau_h$, bbb, bbc, bbs, bbq, bbg, bbe, $bb\mu$, $cccc$, $ccss$, $ccqq$, $ccgg$, $ccee$, $cc\mu\mu$, $cc\tau_h\tau_e$, $cc\tau_h\tau_\mu$, $cc\tau_h\tau_h$, ccb, ccc, ccs, ccq, ccg, cce, $cc\mu$, $ssss$, $ssqq$, $ssgg$, $ssee$, $ss\mu\mu$, $ss\tau_h\tau_e$, $ss\tau_h\tau_\mu$, $ss\tau_h\tau_h$, ssb, ssc, sss, ssq, ssg, sse, $ss\mu$, $qqqq$, $qqgg$, $qqee$, $qq\mu\mu$, $qq\tau_h\tau_e$, $qq\tau_h\tau_\mu$, $qq\tau_h\tau_h$, qqb, qqc, qqs, qqq, qqg, qqe, $qq\mu$, $gggg$, $ggee$, $gg\mu\mu$, $gg\tau_h\tau_e$, $gg\tau_h\tau_\mu$, $gg\tau_h\tau_h$, ggb, ggc, ggs, ggq, ggg, gge, $gg\mu$, bee, cee, see, qee, gee, $b\mu\mu$, $c\mu\mu$, $s\mu\mu$, $q\mu\mu$, $g\mu\mu$, $b\tau_h\tau_e$, $c\tau_h\tau_e$, $s\tau_h\tau_e$, $q\tau_h\tau_e$, $g\tau_h\tau_e$, $b\tau_h\tau_\mu$, $c\tau_h\tau_\mu$, $s\tau_h\tau_\mu$, $q\tau_h\tau_\mu$, $g\tau_h\tau_\mu$, $b\tau_h\tau_h$, $c\tau_h\tau_h$, $s\tau_h\tau_h$, $q\tau_h\tau_h$, $g\tau_h\tau_h$, $qqqb$, $qqqc$, $qqqs$, $bbcq$, $ccbs$, $ccbq$, $ccsq$, $sscq$, $qqbc$, $qqbs$, $qqcs$, $bcsq$, bcs, bcq, bsq, csq, $bce\nu$, $cse\nu$, $bqe\nu$, $cqe\nu$, $sqe\nu$, $qqe\nu$, $bc\mu\nu$, $cs\mu\nu$, $bq\mu\nu$, $cq\mu\nu$, $sq\mu\nu$, $qq\mu\nu$, $bc\tau_e\nu$, $cs\tau_e\nu$, $bq\tau_e\nu$, $cq\tau_e\nu$, $sq\tau_e\nu$, $qq\tau_e\nu$, $bc\tau_\mu\nu$, $cs\tau_\mu\nu$, $bq\tau_\mu\nu$, $cq\tau_\mu\nu$, $sq\tau_\mu\nu$, $qq\tau_\mu\nu$, $bc\tau_h\nu$, $cs\tau_h\nu$, $bq\tau_h\nu$, $cq\tau_h\nu$, $sq\tau_h\nu$, $qq\tau_h\nu$
QCD jets	161–187	$bbccss$, $bbccs$, $bbcc$, $bbcss$, $bbcs$, bbc, $bbss$, bbs, bb, $bccss$, $bccs$, bcc, $bcss$, bcs, bc, bss, bs, b, $ccss$, ccs, cc, css, cs, c, ss, s, others

resulting to 4-prong or 3-prong

All final states!

Key property: we do not focus on any specific *X* and *Y* masses
Their masses are variables: ranges from 20-500 GeV

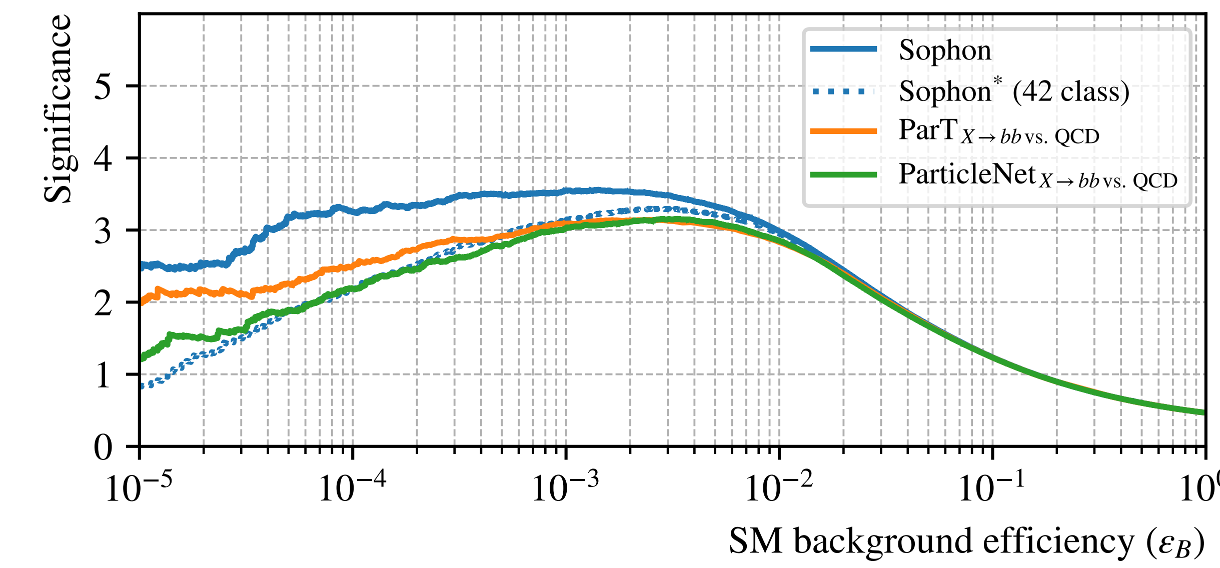
Sophon: performance benchmark

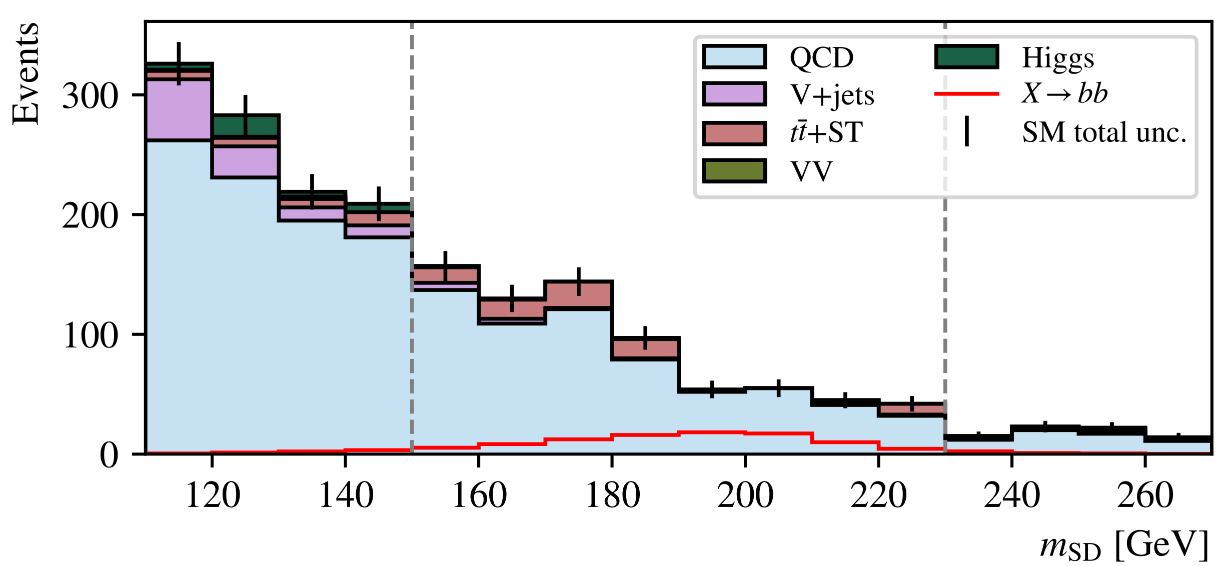
arXiv:2405.12972

Search significance:

$Z = \sqrt{2((s+b)\log(1+s/b)-s)}$

Direct tagging ability





- Apply tagger selection
- Check discrimination power of
  X (200 GeV) → **bb** signal vs. all backgrounds

- **Sophon** (training on 188 classes) has best performance

$$\text{discr}(X \to bb \text{ vs. QCD}) = \frac{g_{X\to bb}}{g_{X\to bb} + \sum_{l=1}^{27} g_{\text{QCD}_l}}$$

- Performance gain does come from large-scale classification (compared to **Sophon* (42 classes)**)
- **ParT** and **ParticleNet** for binary classification: they represent the best performance we can reach in experiment now

Sophon: performance benchmark

arXiv:2405.12972

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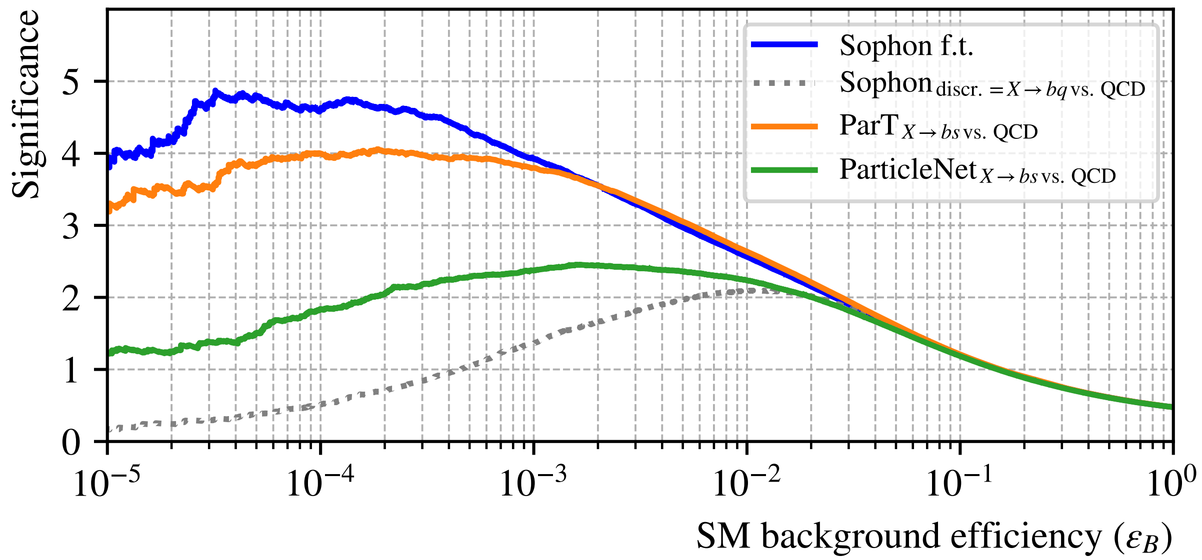
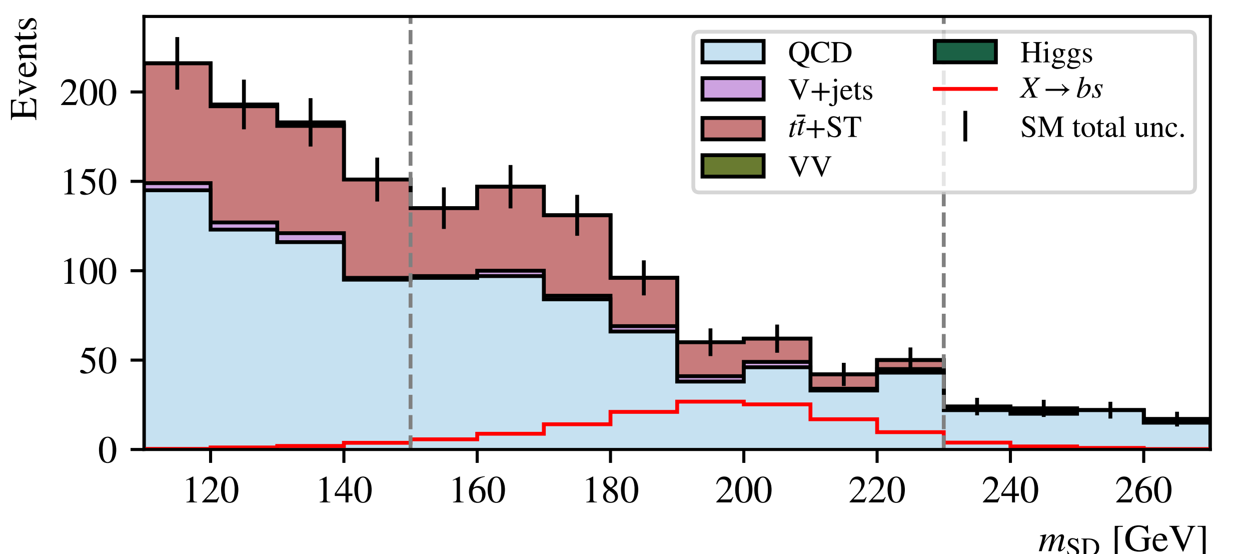




- Check discrimination power of X (200 GeV) → **bs** signal vs. all backgrounds

Transfer learning ability

(adapt it to a brand new task)

- **Sophon** (training on 188 classes) reaches the best performance **after fine-tuned (via transfer learning)**
- **ParT** and **ParticleNet** for binary X→bs vs QCD classification: they reveal the best performance we can reach in the experiment now

Sophon: close to real experimental performance?

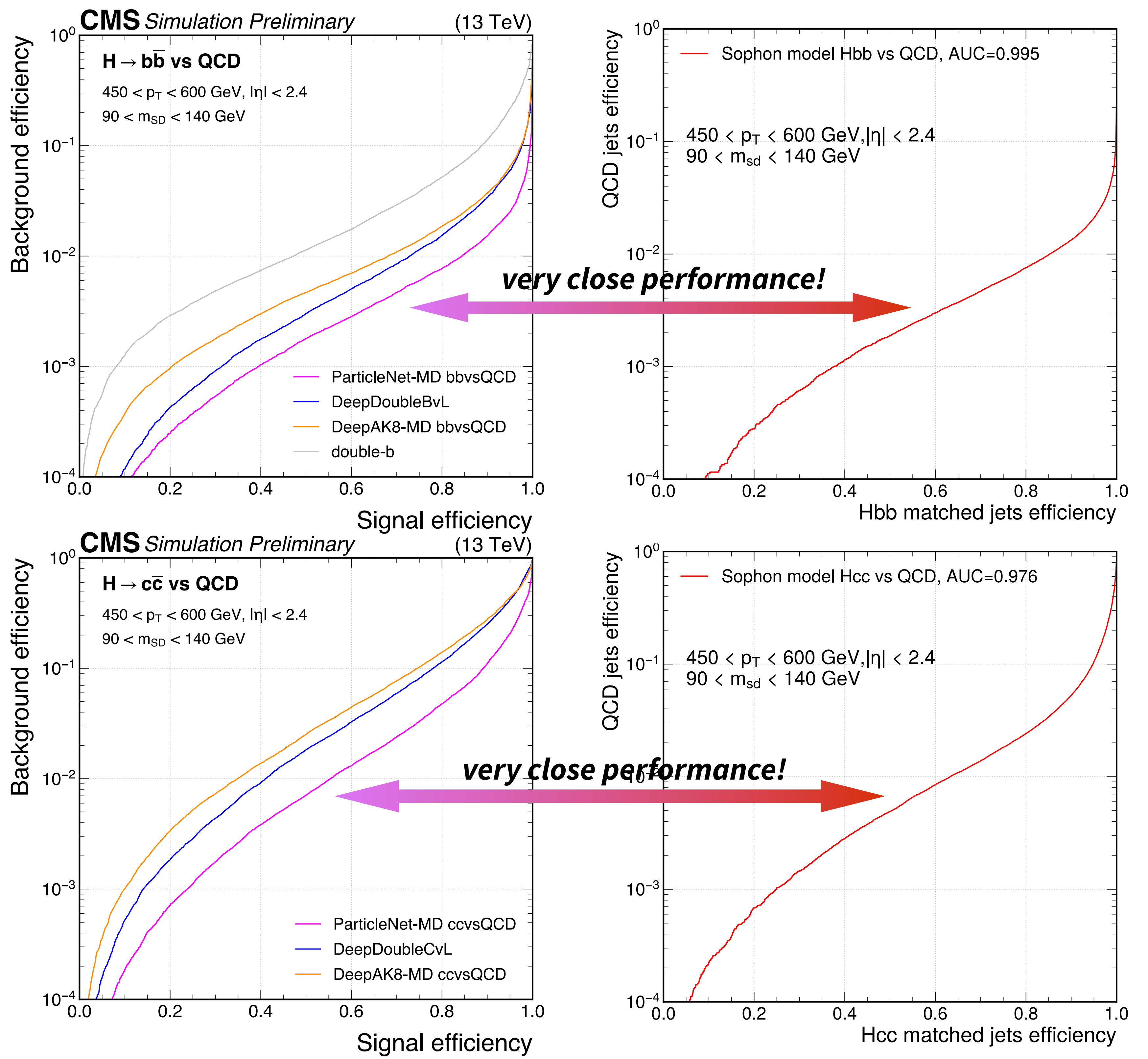
Thanks Yuzhe for his input

Take recent **CMS performance plots** as an example

Benchmark performance on SM H→$b\bar{b}$/$c\bar{c}$ jets vs QCD background jets

- Demonstrate that **applying "Sophon" on Delphes dataset for pheno study** is pretty realistic

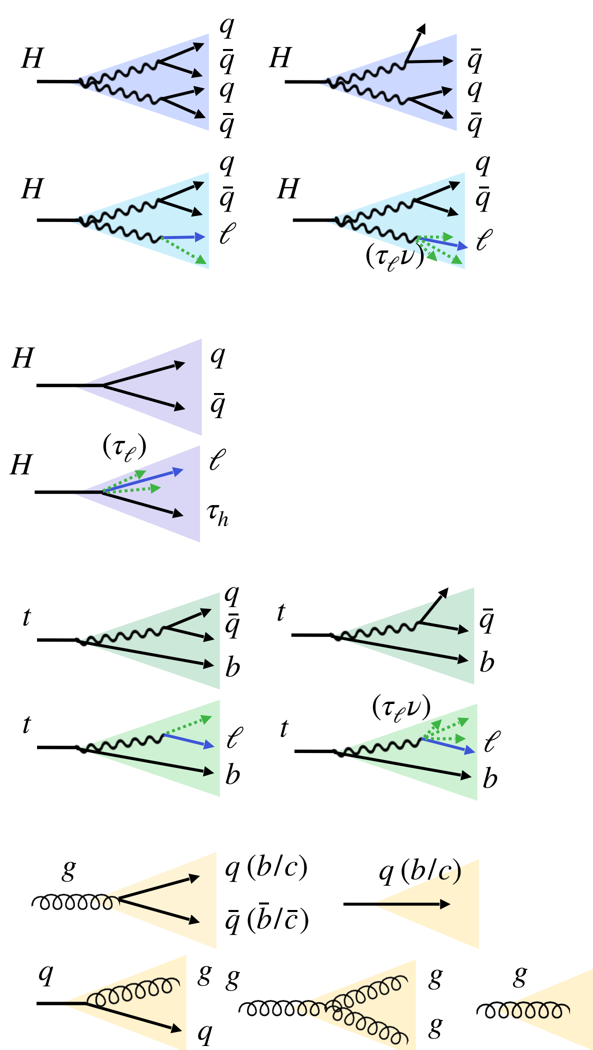
CMS results CMS-PAS-BTV-22-001 ***Sophon results*** *(on Delphes dataset)*



Highlight: CMS's Global ParT tagger

CMS-PAS-HIG-23-012

Process	Final state/ prongness	heavy flavour	# of classes
H→VV (full-hadronic)	qqqq	0c/1c/2c	3
	qqq		3
H→WW (semi-leptonic)	eνqq	0c/1c	2
	μνqq		2
	τ_eνqq		2
	τ_μνqq		2
	τ_hνqq		2
H→qq		bb	1
		cc	1
		ss	1
		qq (q=u/d)	1
H→ττ	$\tau_e\tau_h$		1
	$\tau_\mu\tau_h$		1
	$\tau_h\tau_h$		1
t→bW (hadronic)	bqq	1b + 0c/1c	2
	bq		2
t→bW (leptonic)	beν	1b	1
	bμν		1
	bτ_eν		1
	bτ_μν		1
	bτ_hν		1
QCD		b	1
		bb	1
		c	1
		cc	1
		others (light)	1



A global large-*R* mass-decorrelated tagger for **37-category classification**

- First time identifying the H→WW→4q signature with a jet tagger
- set a strong limit to κ_{2V} in the search of HH→bbVV signal

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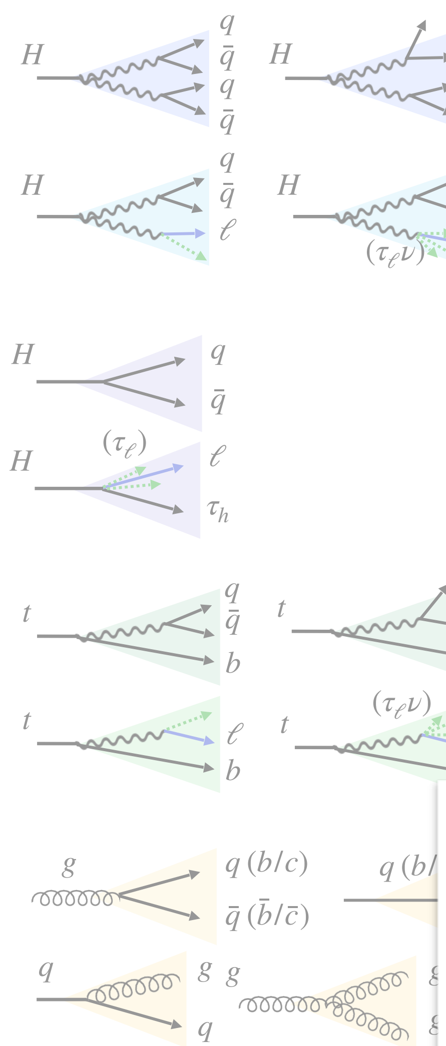
	τ_eνqq		2
	τ_μνqq		2
	τ_hνqq		2
H→qq		bb	1
		cc	1
		ss	1
		qq (q=u/d)	1
H→ττ	$\tau_e\tau_h$		1
	$\tau_\mu\tau_h$		1
	$\tau_h\tau_h$		1
t→bW (hadronic)	bqq	1b + 0c/1c	2
	bq		2
t→bW (leptonic)	beν	1b	1
	bμν		1
	bτ_eν		1
	bτ_μν		1
	bτ_hν		1
QCD		b	1
		bb	1
		c	1
		cc	1
		others (light)	1



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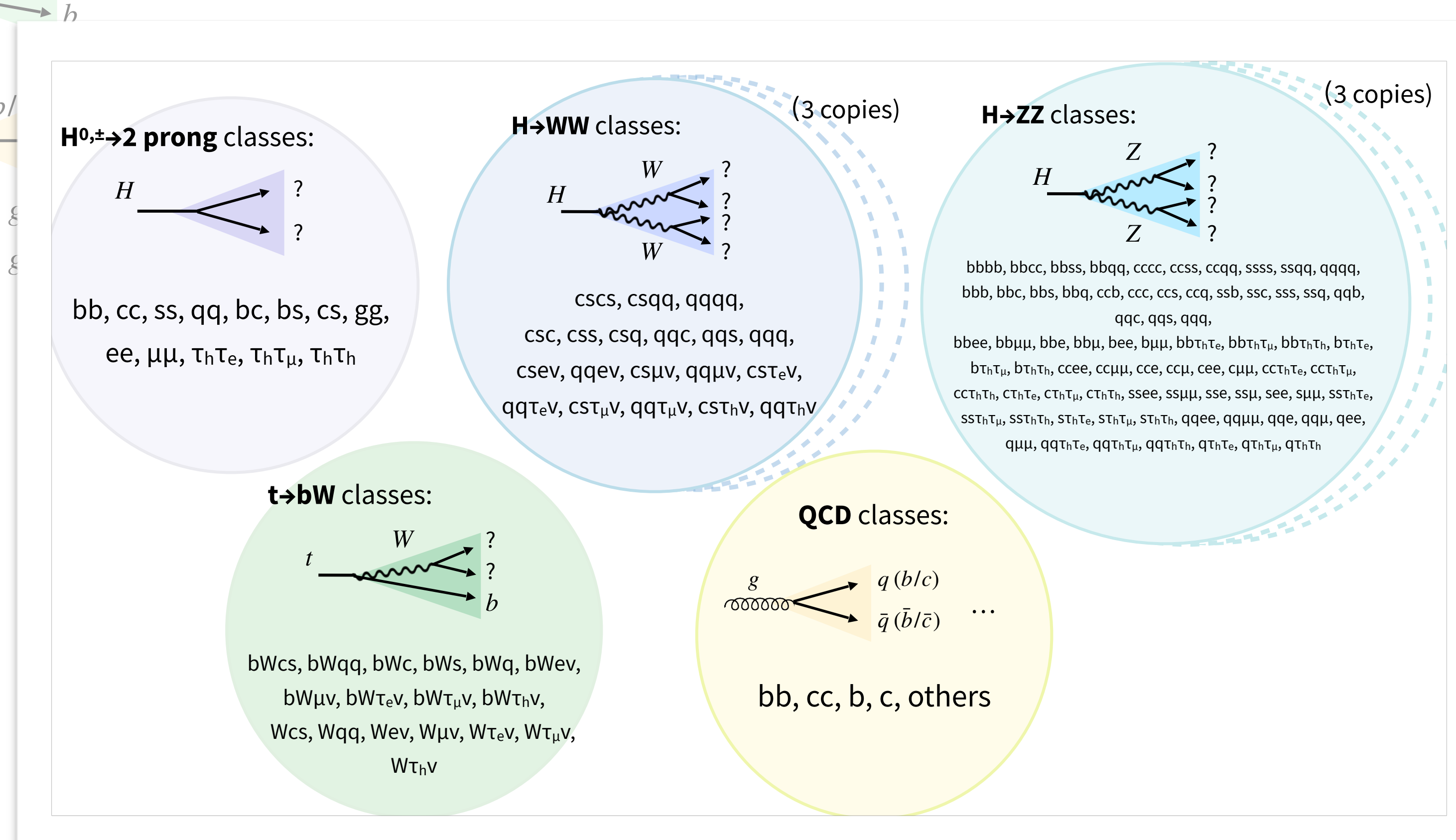
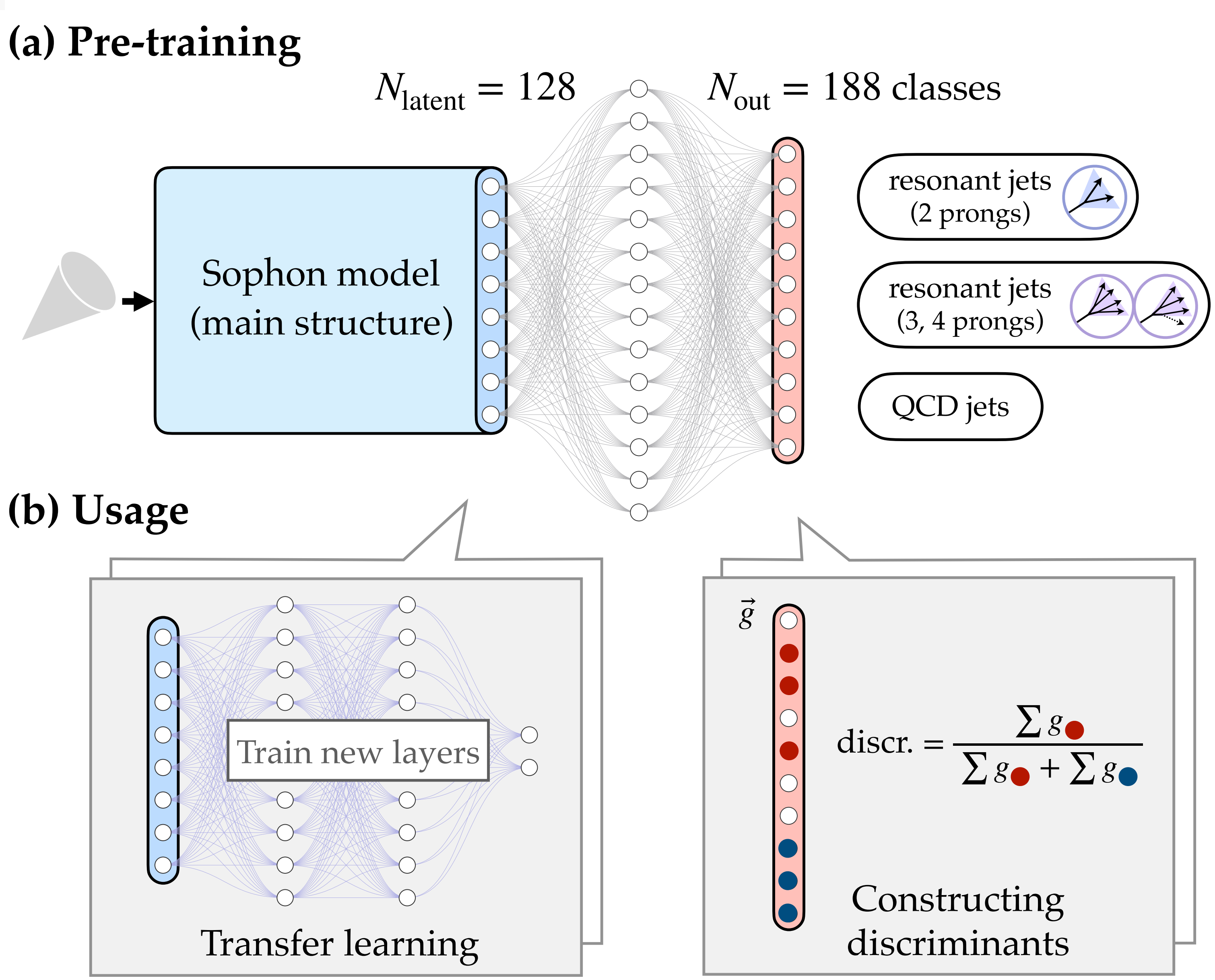


and we plan to update the CMS tagger under Sophon's philosophy

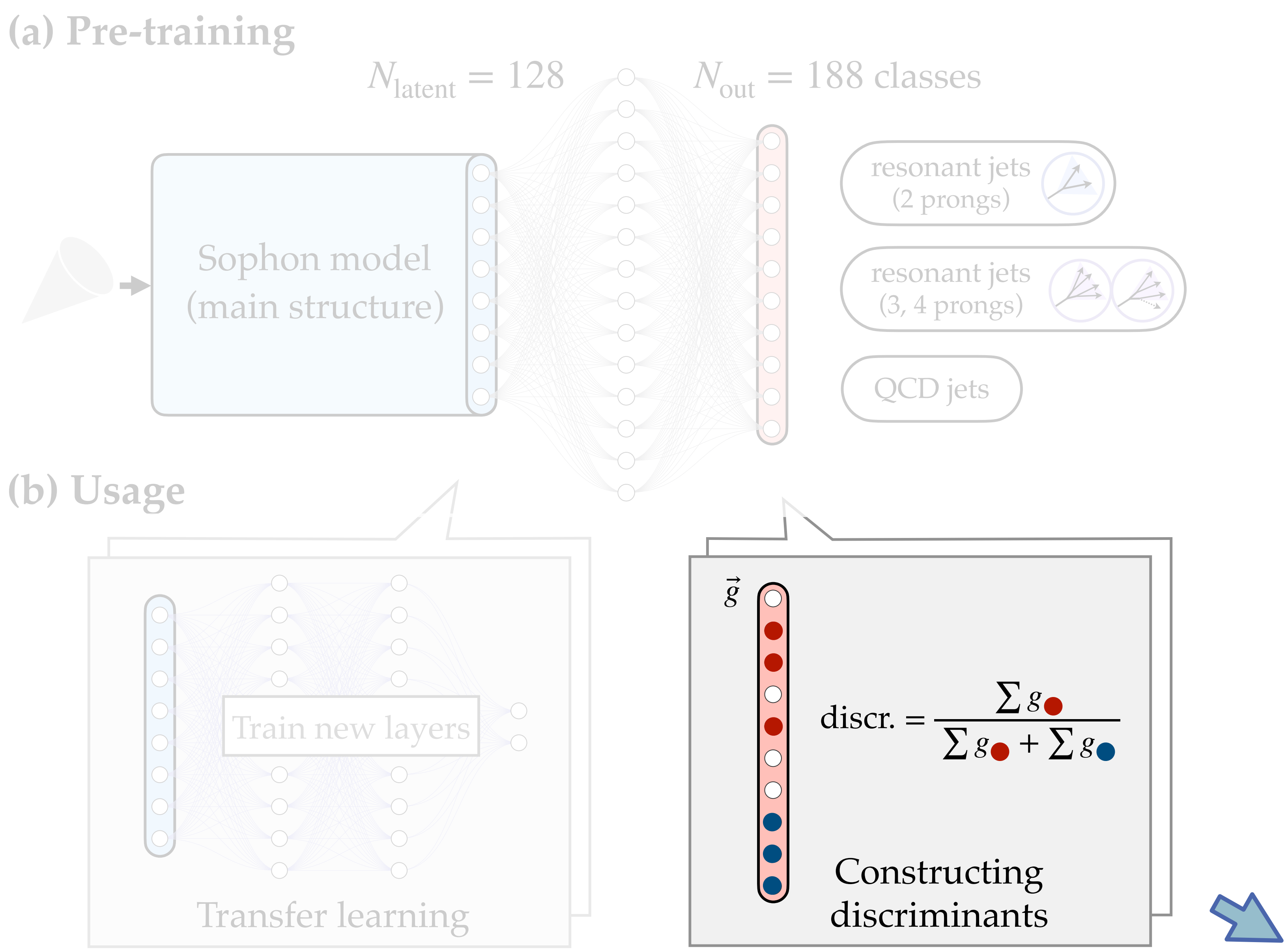
please stay tuned!

Implications for LHC resonance search

Using Sophon



Using Sophon

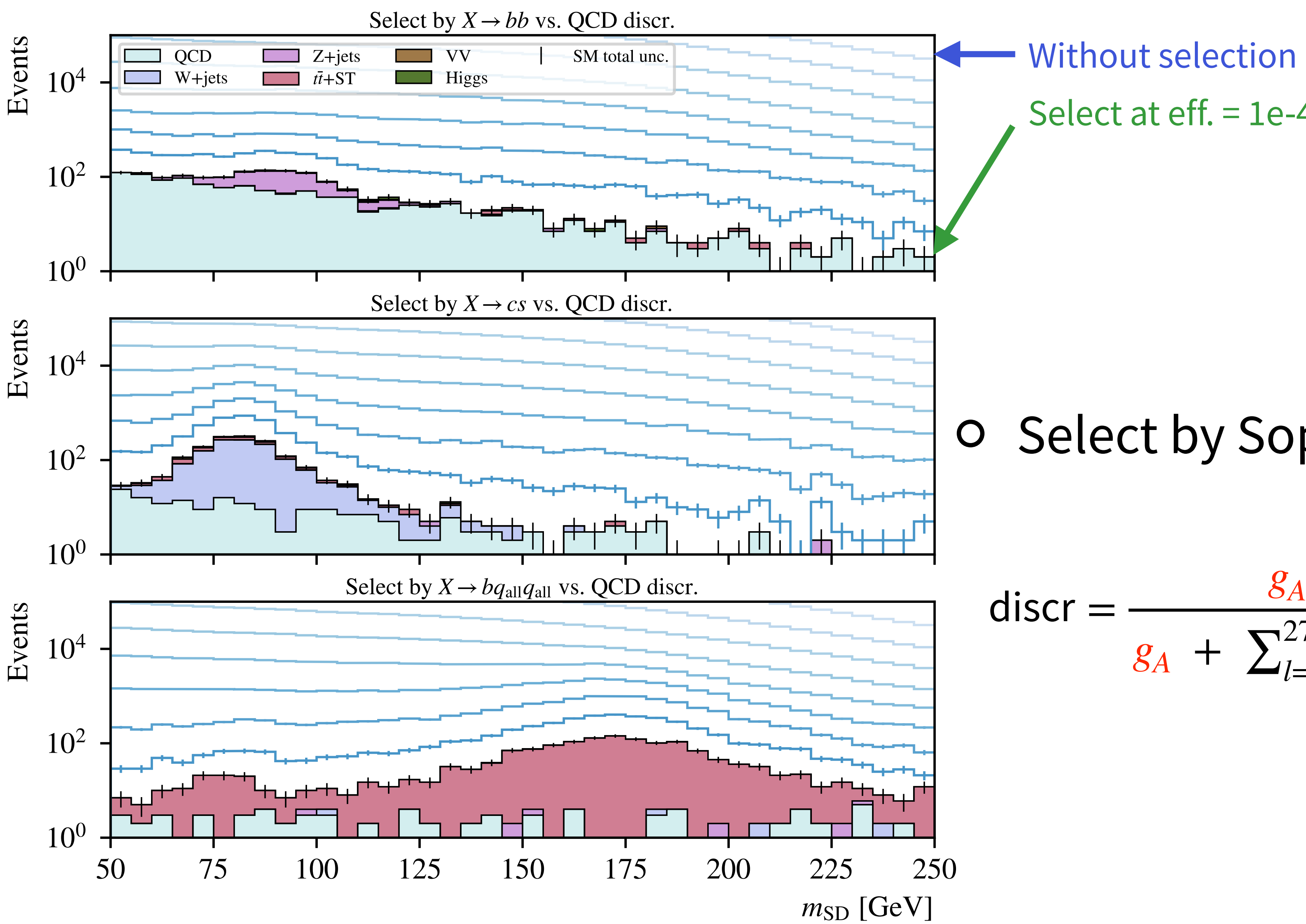


Use it out of the box!

Construct a dedicated discr.
→ perform a bump hunt

Can we rediscover the SM particles?

- ➔ Simulate 40fb^{-1} LHC collision events, $\sqrt{s}$ = 13 TeV, nPU=50
  - focus on the large-*R* jet trigger (triggered with Σp_T threshold and trimmed mass)
  - abundant QCD backgrounds
  - **rediscover Z/W/t particles** simply from the large-*R* jet's **mass spectrum**

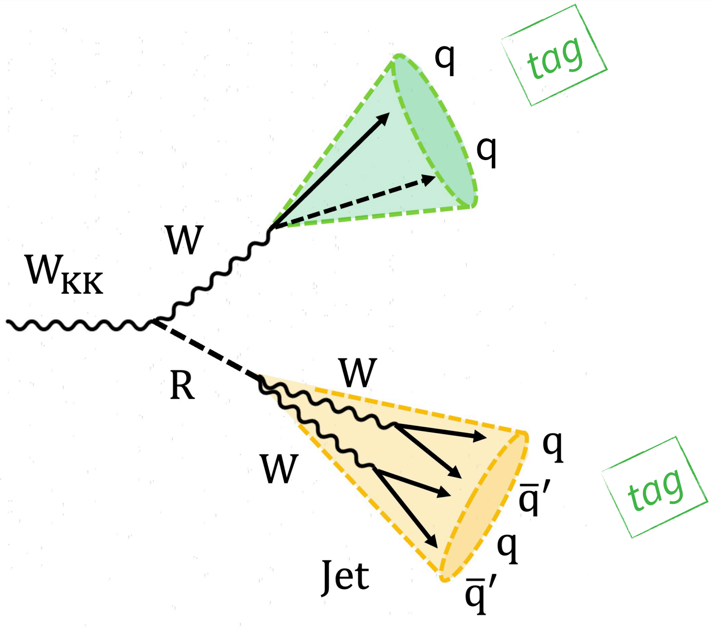


- Select by Sophon's different discriminants

$$\mathrm{discr} = \frac{g_A}{g_A + \sum_{l=1}^{27} g_{\mathrm{QCD}_l}} \quad \begin{cases} ①: A = \{bb\} \\ ②: A = \{cs\} \\ ③: A = \{ccb, ssb, qqb, \\ \quad bcs, bcq, bsq\} \end{cases}$$

More heavy resonances

- Consider triboson signal:
  W' ($m_{W'}$ = 3 TeV) → $W\phi$ (m_ϕ = 400 GeV) → WWW (fully hadronic decays)
- Optimize an event-level discr. from tagger discr.



$$\text{discr} = \sum_{\text{jet}=1,2} \frac{g_{A,\text{jet}}}{g_{A,\text{jet}} + \sum_{l=1}^{27} g_{\text{QCD}_l,\text{jet}}}$$ (sum for jets 1, 2)

$$A = \begin{cases} 0.3 \times \{cs, qq\} \\ +\ 0.1 \times \{ccss, qqcs, qqqq\} \\ +\ 0.6 \times \{ccs, ccq, ssc, ssq, qqc, qqs, qqq\} \end{cases}$$

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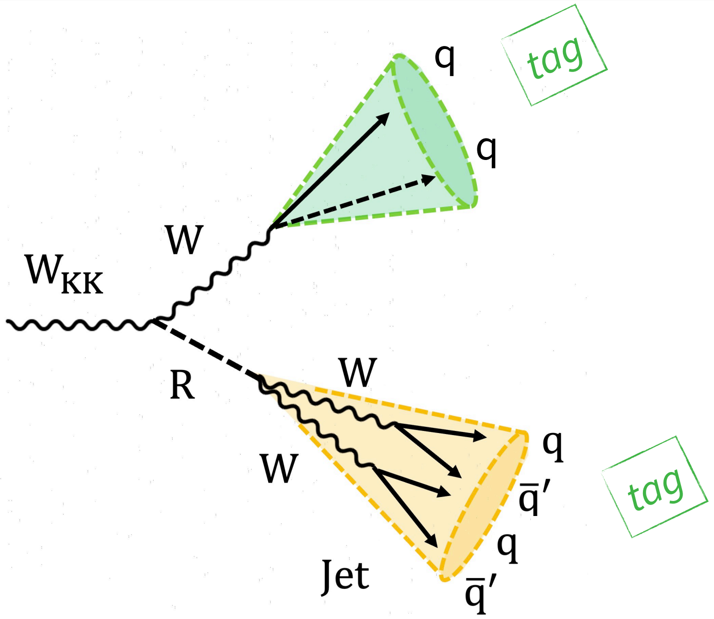


- Optimize an event-level discr. from tagger discr.

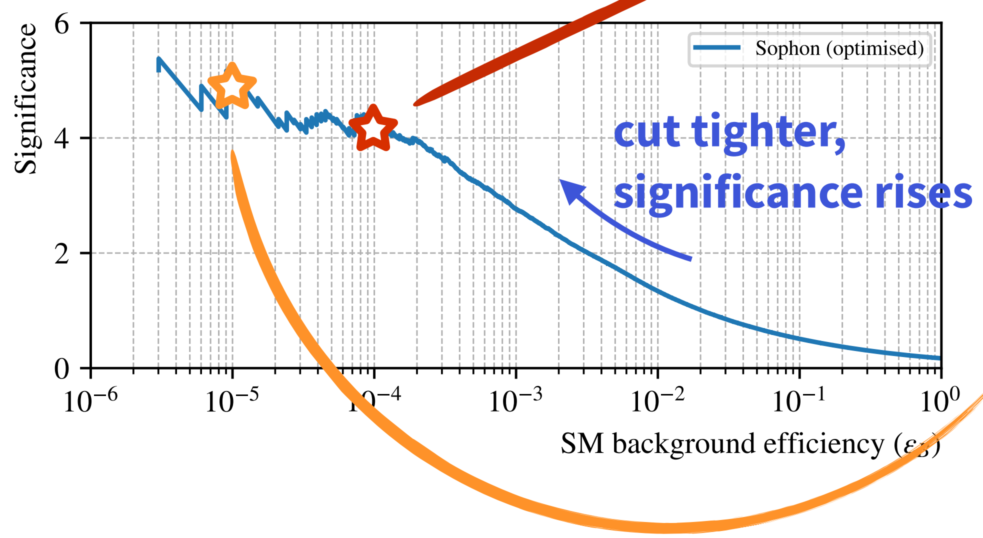
$$\text{discr} = \sum_{\text{jet}=1,2} \frac{g_{A,\text{jet}}}{g_{A,\text{jet}} + \sum_{l=1}^{27} g_{\text{QCD}_l,\text{jet}}}$$ (sum for jets 1, 2)

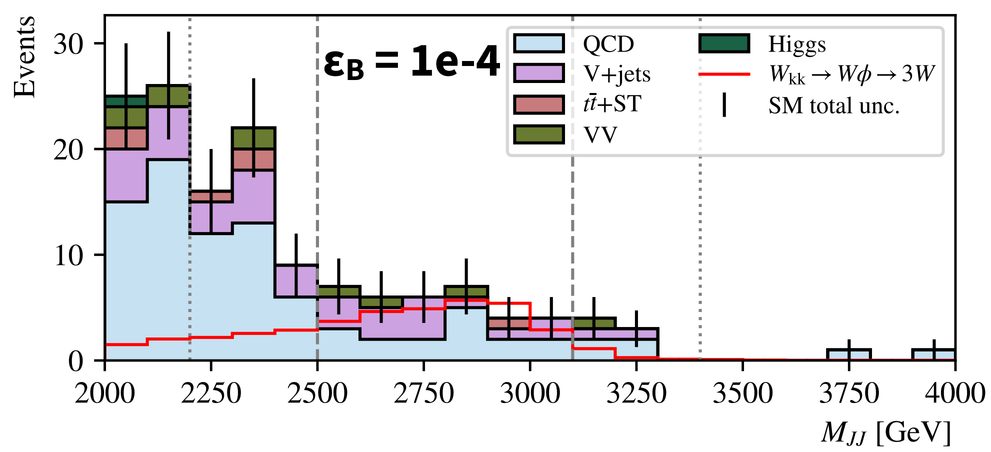
$$A = \begin{cases} 0.3 \times \{cs, qq\} \\ + 0.1 \times \{ccss, qqcs, qqqq\} \\ + 0.6 \times \{ccs, ccq, ssc, ssq, qqc, qqs, qqq\} \end{cases}$$

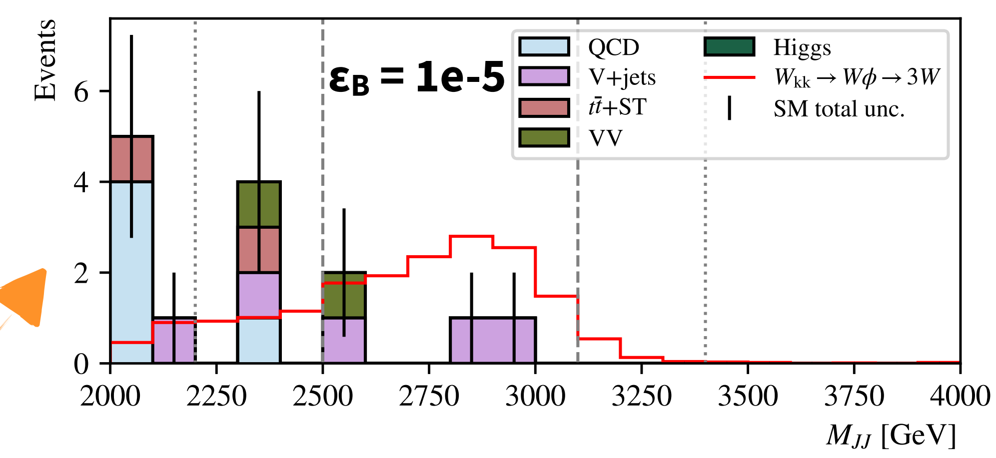
Search significance

$$Z = \sqrt{2((s+b)\log(1+s/b) - s)}$$

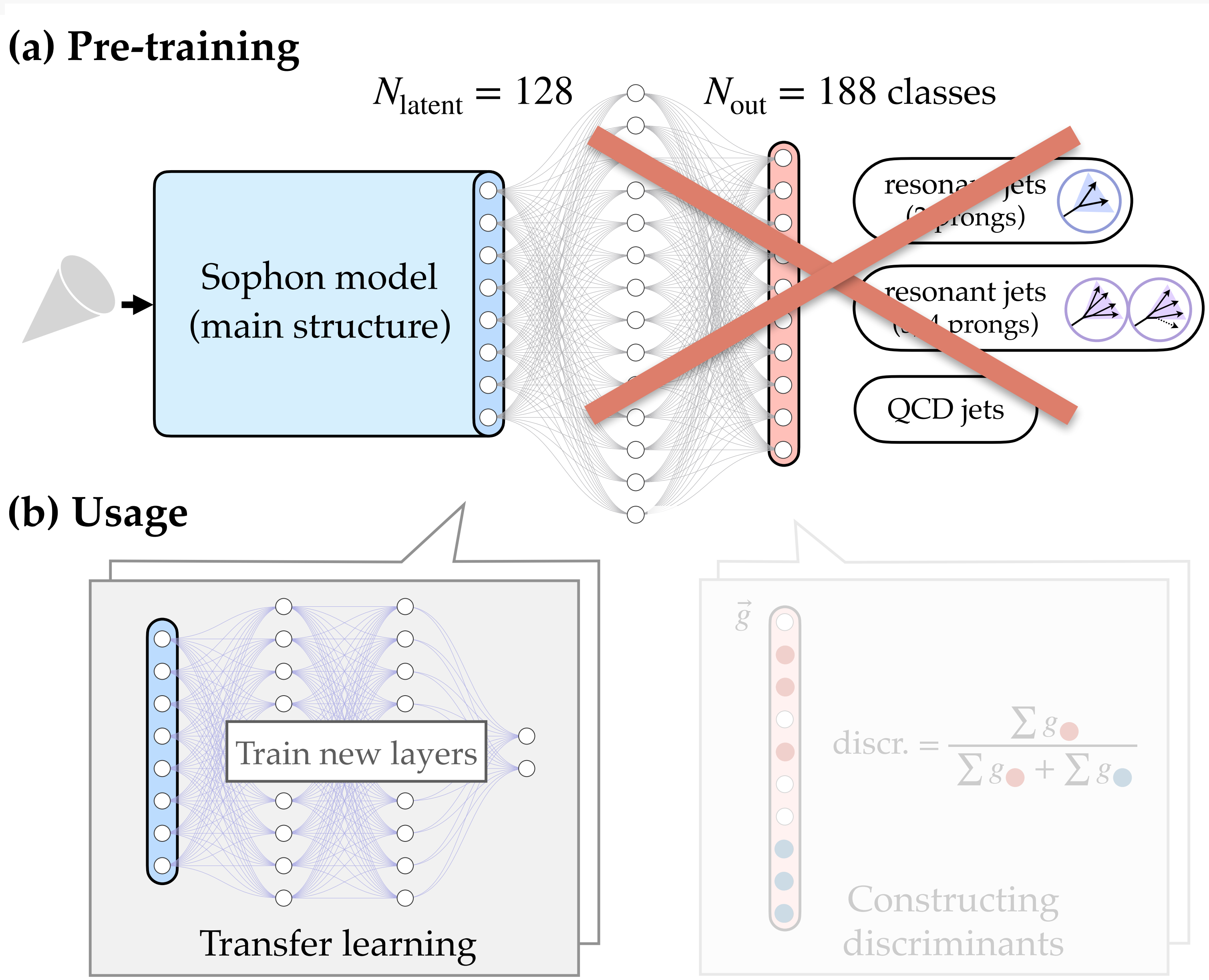
in dijet inv. mass window **2500–3100 GeV**







Sophon's transfer learning



- Transfer to uncovered tagging scenarios…
- facilitate anomaly detection (weakly-supervised, autoencoder)…
- *more potential to unlock!*

Use it out of the box!

Construct a dedicated discr.
→ perform a bump hunt

Background: anomaly detection in weakly-supervised approach

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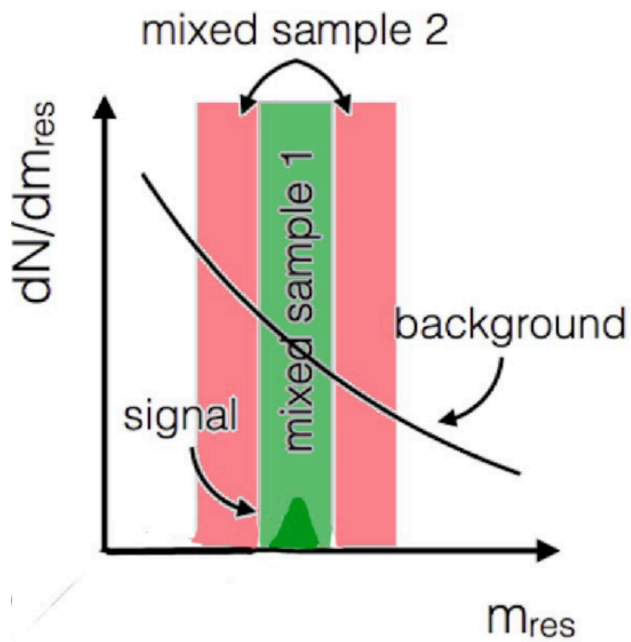

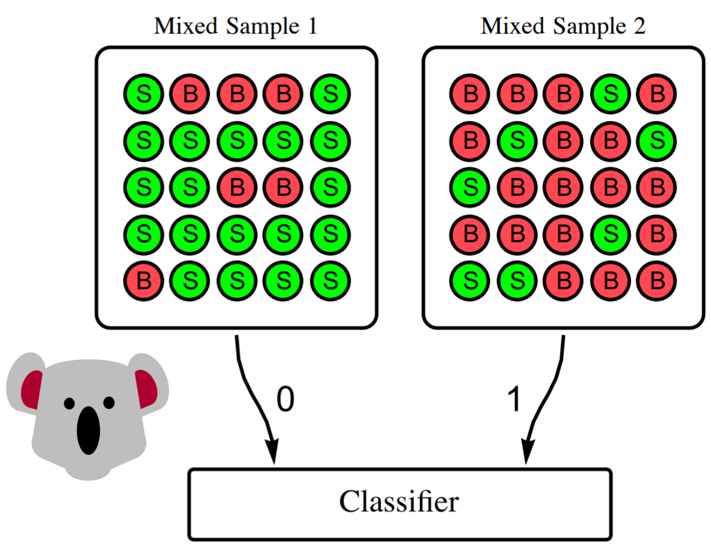

Equivalent effect for training **S** vs **B**

➔ Recall the early work: CWoLa (classification without labels) Hunting

- allow to detect anomalies purely from data
- train a classifier for mass window vs mass sideband (mixed sample 1 vs 2)
- many improved approaches in recent years → very active field

Background: anomaly detection in weakly-supervised approach

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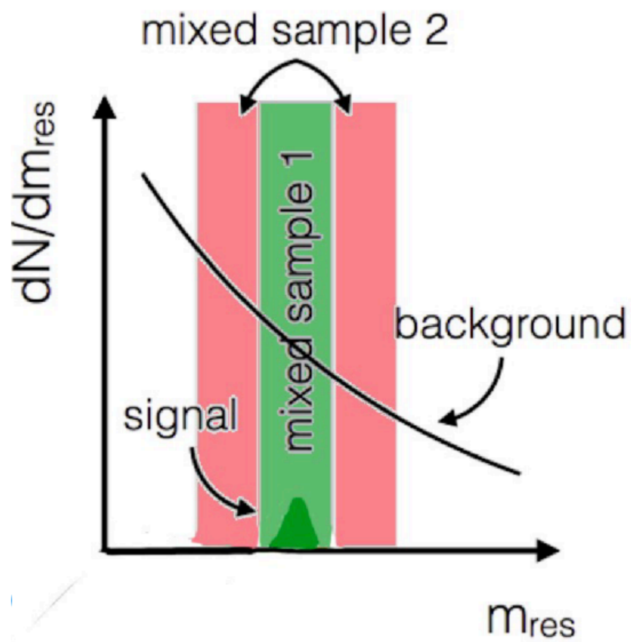

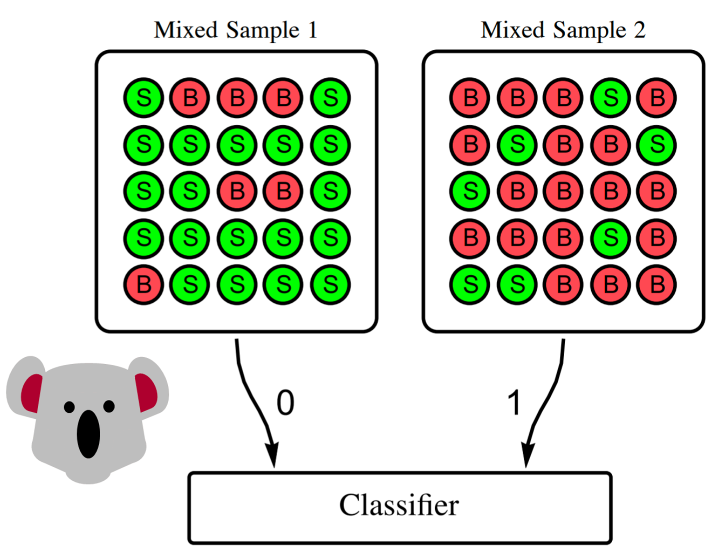

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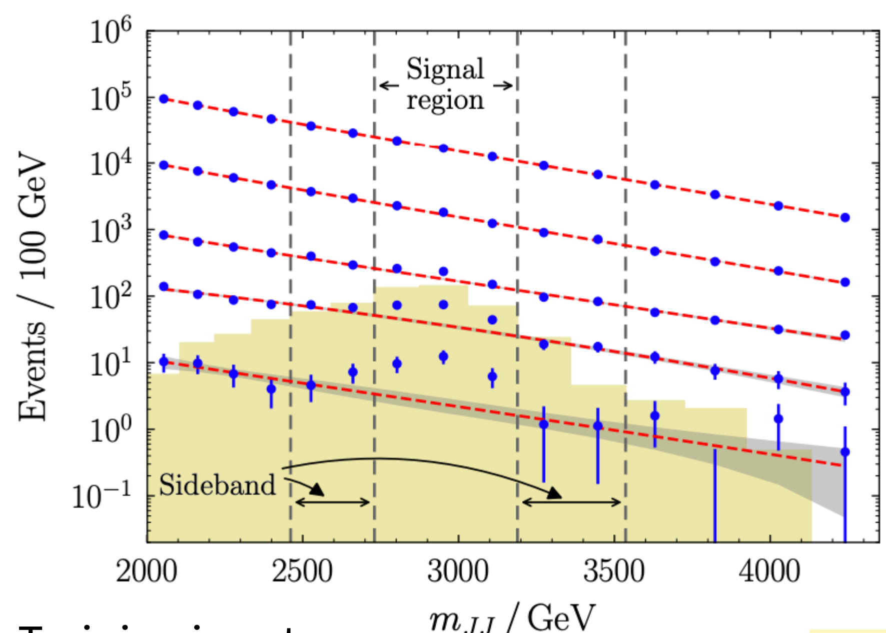
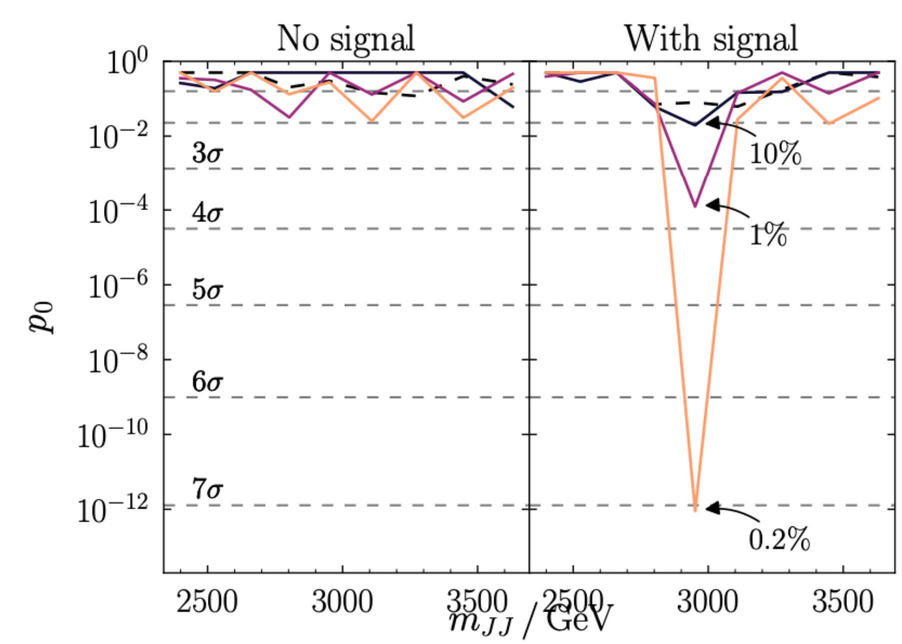


Training input

$m_J, \sqrt{\tau_1^{(2)}/\tau_1^{(1)}}, \tau_{21}, \tau_{32}, \tau_{43}, n_{\mathrm{trk}},$

can discover $W' \to W\phi \to WWW$ signals

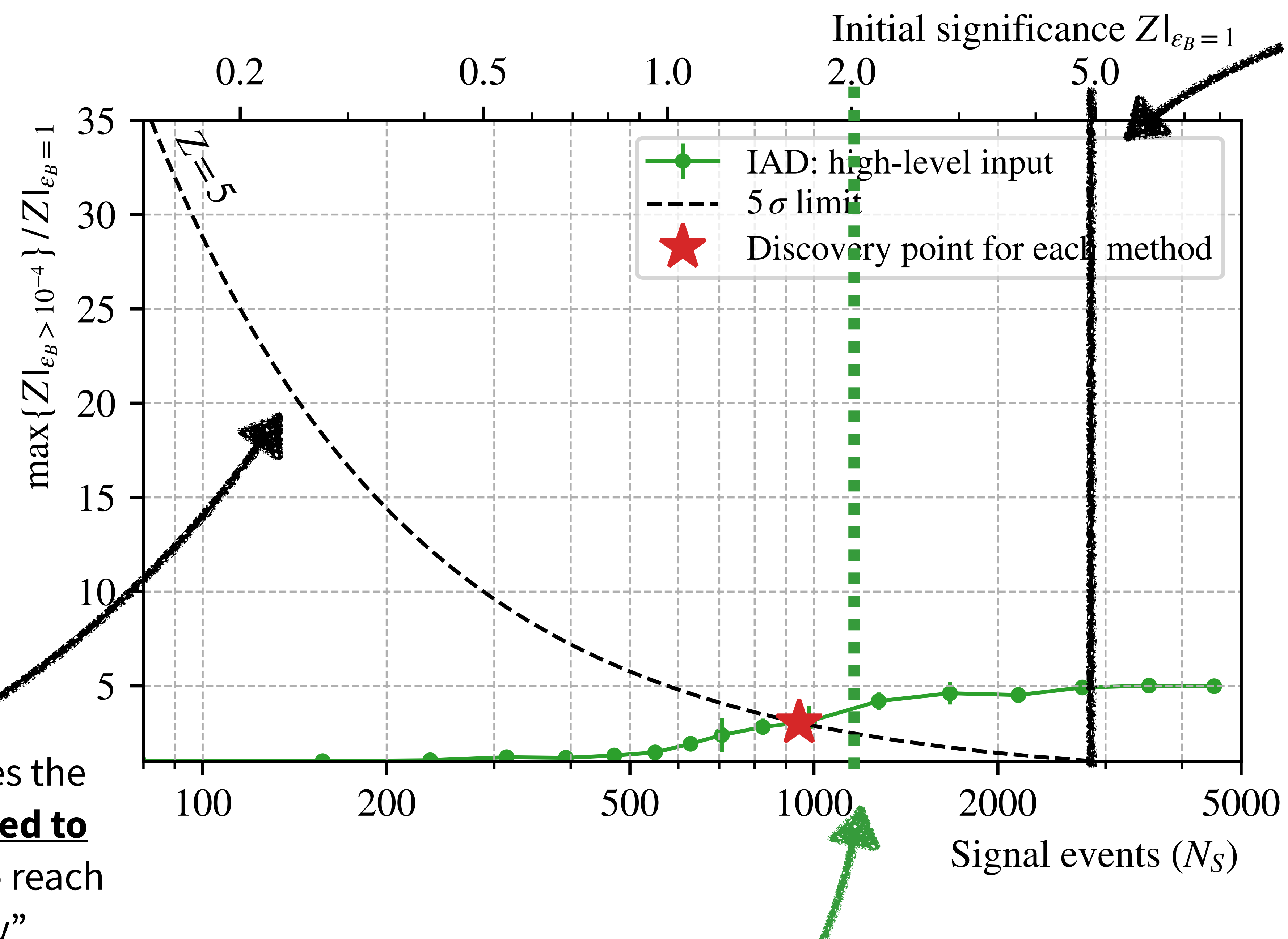
see 2σ → 7σ improvement



PRL, 121 (2018) 24, 241803

PRD, 99 (2019) 1, 014038

Dijet search capabilities

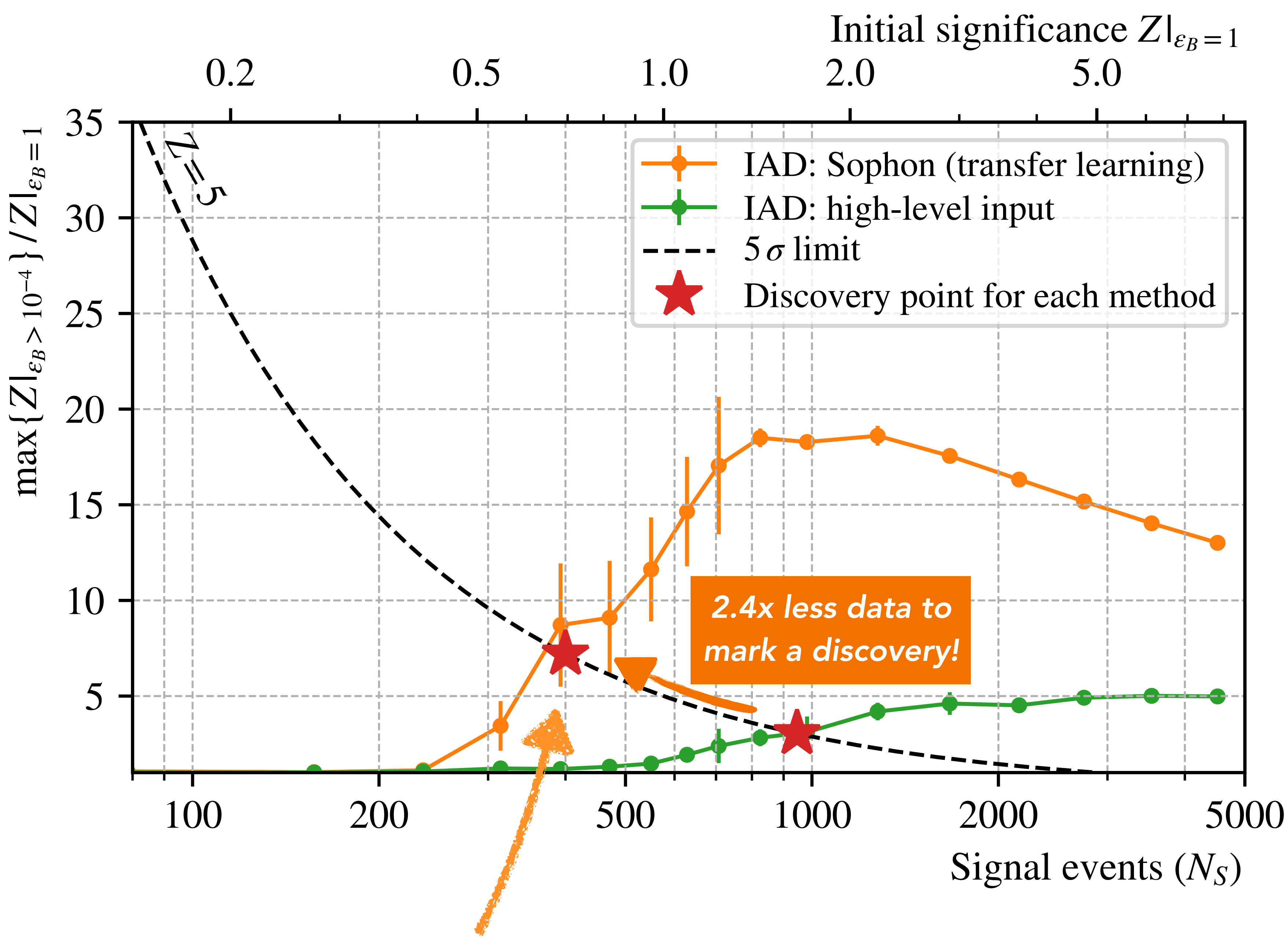


"If signal events reach this point, **with initial *Z*=5**, then we have already discovered the signal without needing to make a cut"

"How much does the **significance need to be increased** to reach the 5σ discovery"

a similar 2σ→7σ is reached with conventional AD approach; ~reproduce the result in *PRL, 121 (2018) 24, 241803*

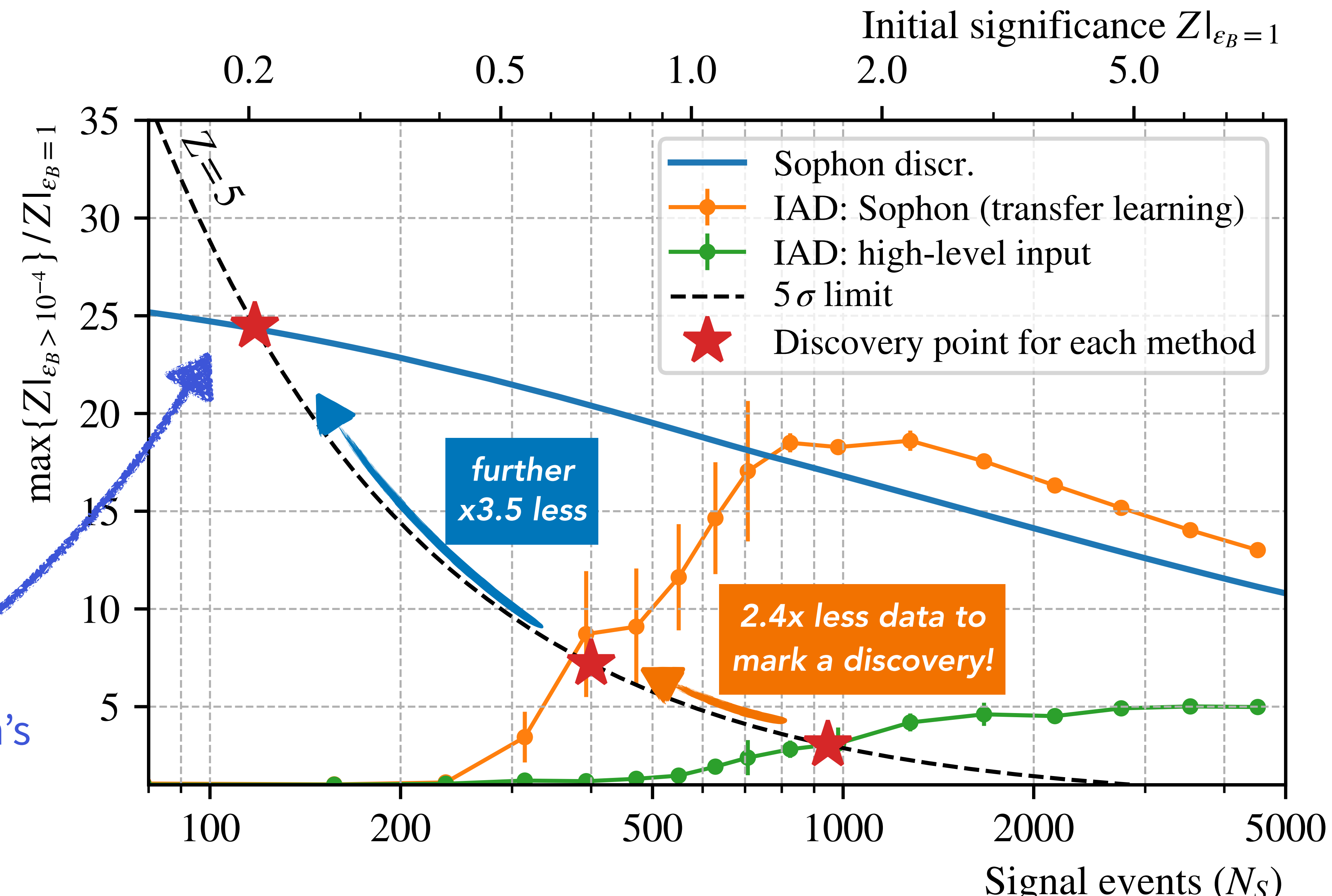
Dijet search capabilities



Combining Sophon's transfer learning (using Sophon's "knowledge") with AD marks a success

- More sensitive to low signal (**even starting at ~0.6σ**)
- Much improved S vs B distinguishability than using high-level input

Dijet search capabilities



using Sophon's constructed discriminant

$$\text{discr} = \sum_{\text{jet}=1,2} \frac{g_{A,\text{jet}}}{g_{A,\text{jet}} + \sum_{l=1}^{27} g_{\text{QCD}_l,\text{jet}}}$$

$$A = \begin{cases} 0.3 \times \{cs, qq\} \\ + 0.1 \times \{ccss, qqcs, qqqq\} \\ + 0.6 \times \{ccs, ccq, ssc, ssq, qqc, qqs, qqq\} \end{cases}$$

Summary and outlook

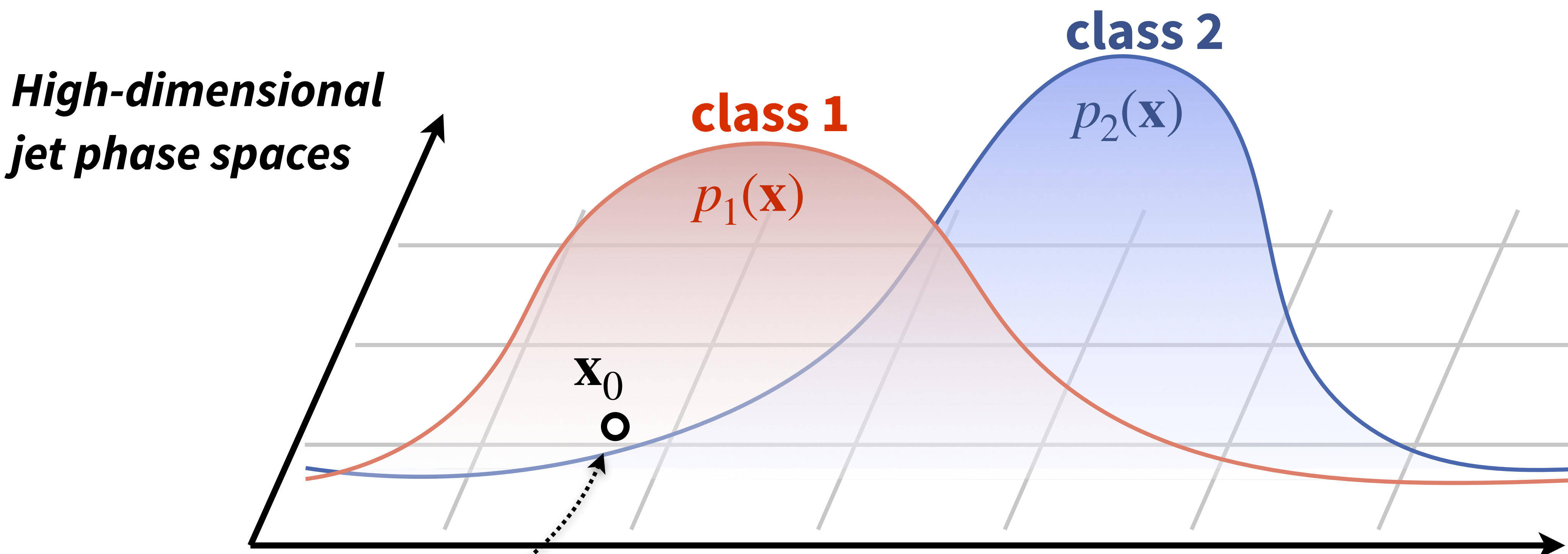
arXiv:2405.12972

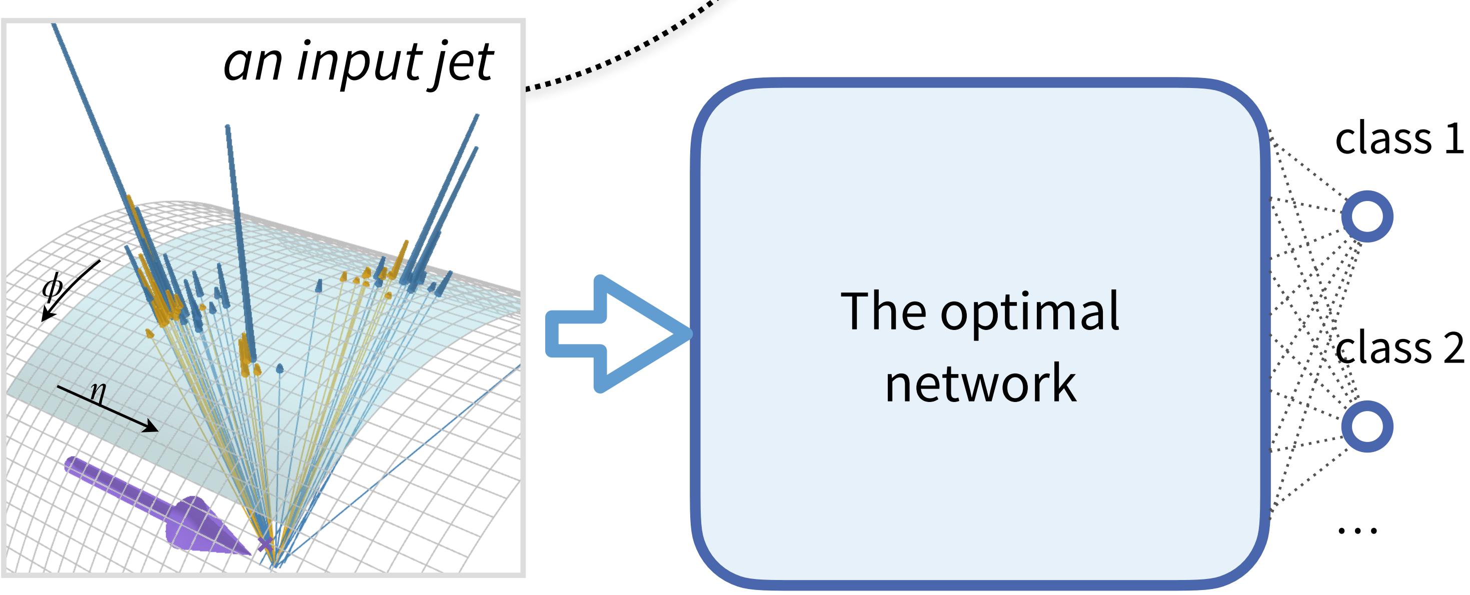
- Sophon releases a lot of new opportunities for future LHC experiments
  - simply viewed as a **"global large-*R* jet tagger"** → should bring benefits of the advanced NN to ~all hadronic final-state searches
  - also viewed as a pre-trained jet model: a foundation model tailored for LHC analyses
- Proposed the **JetClass-II** dataset and the **Sophon** model
  - **JetClass-II** covers more comprehensive phase spaces and can be a good playground to develop future foundation models
  - the **Sophon** model can be helpful in delivering future LHC pheno research! [see implementation details on our Github repo]
    - optimizing sensitivity for dedicated searches/anomaly detection/novel paradigms…
  - this work demonstrates that it can be a great booster to LHC's broad resonance search programs
- Stay tuned to their applications to real LHC experiments!

Backup

Statistical essence of jet tagging problem

- **Question: where is the limit of jet tagging?**
- Answer: the probability density ratio of two classes provides the optimal tagging



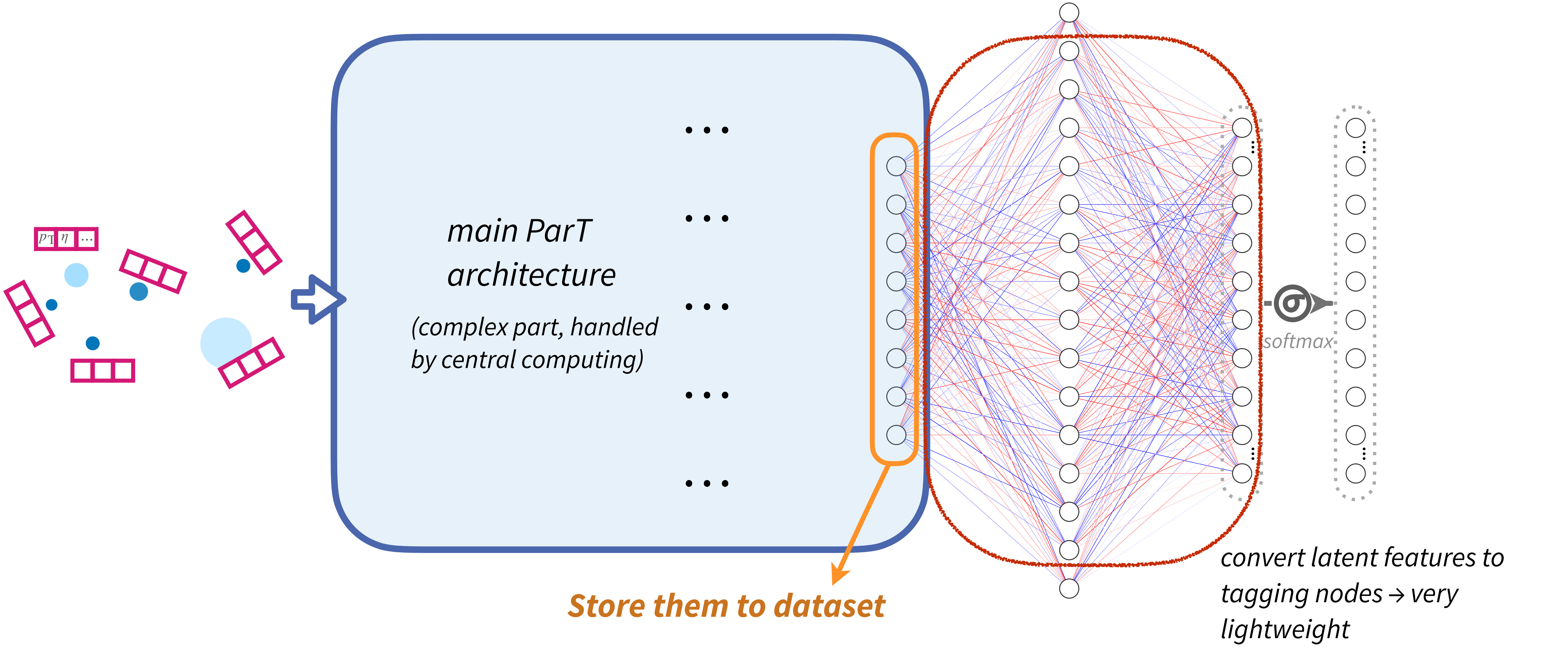


- Ideal classifier network results in $g_1 : g_2 : \ldots = p_1(\mathbf{x}_0) : p_2(\mathbf{x}_0) : \ldots$
- It is a direct estimation of p
- The **network capacity** decides how close the estimation is

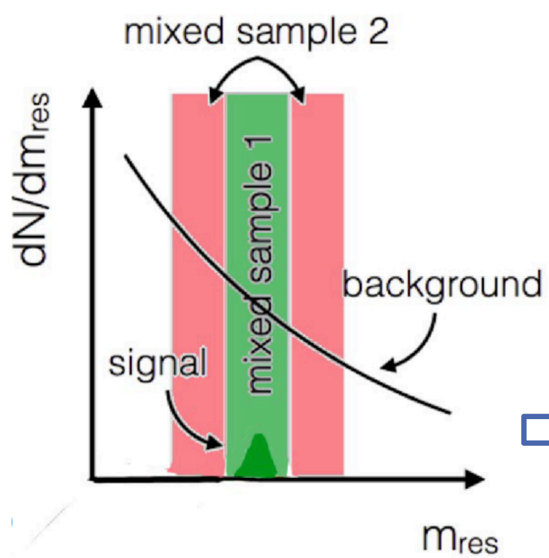
How to deploy the model to LHC experiments?

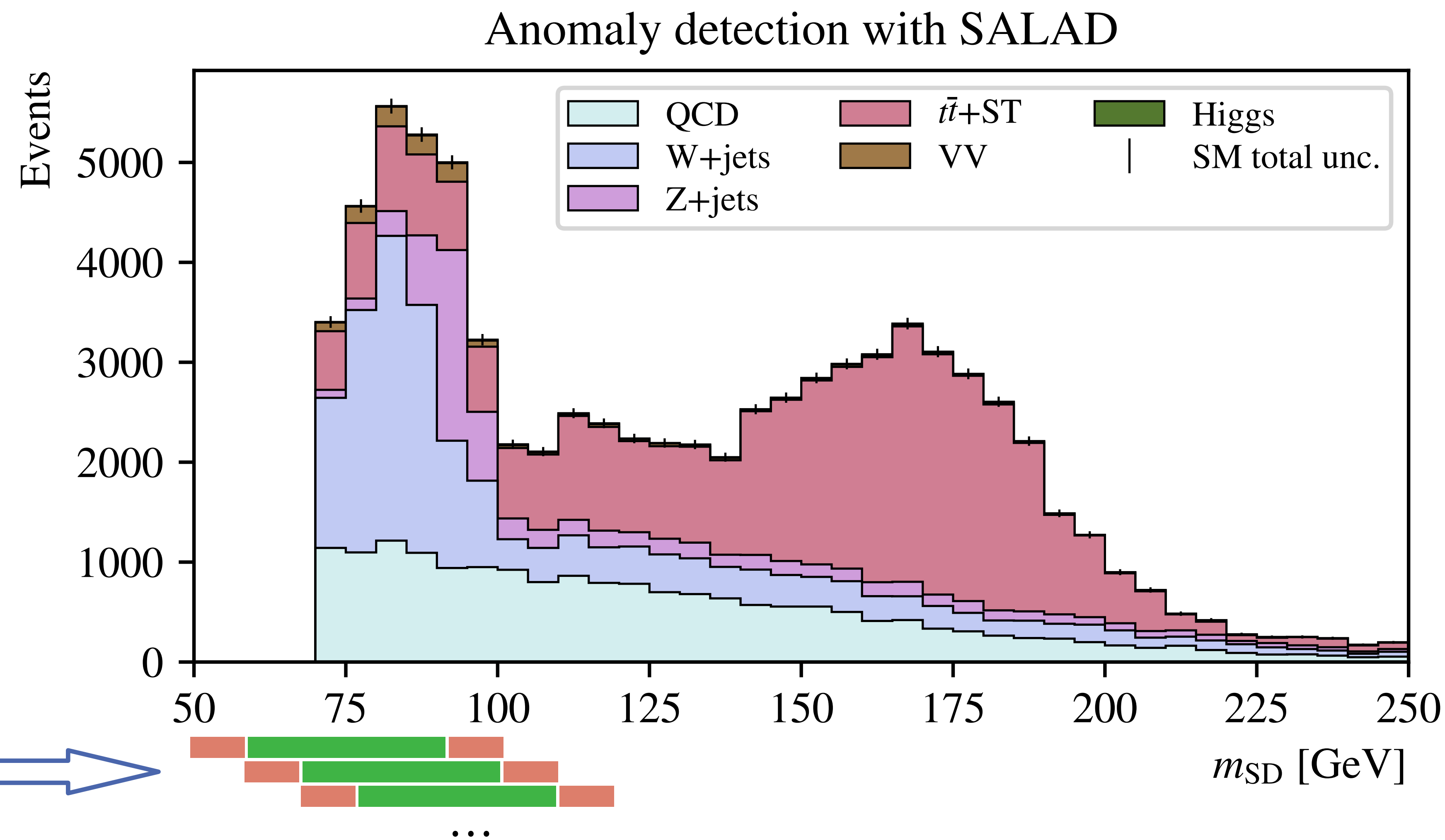
→ Implies how we can do future analysis

- hidden layer neurons values are stored in official sample
- analysis can use them for fine-tuning (equivalently, just think that they are special jet variables)
- easy to implement & integrate into existing workflow



Sophon's transfer learning × anomaly detection





➔ Do SALAD (similar to CWOLA Hunt) in each sliding window

- ❖ purify those peculiar jets in that mass window

➔ Sophon's latent space has encoded fruitful knowledge on "final-state properties"