

Unravelling the origins of top pairs: production mode analysis in ATLAS

DESY Summer School Program project

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ATLAS group

Supervised by: *K. Behr, E. Jones, M. Gonzalez, F. Jolly*

02/09/2025

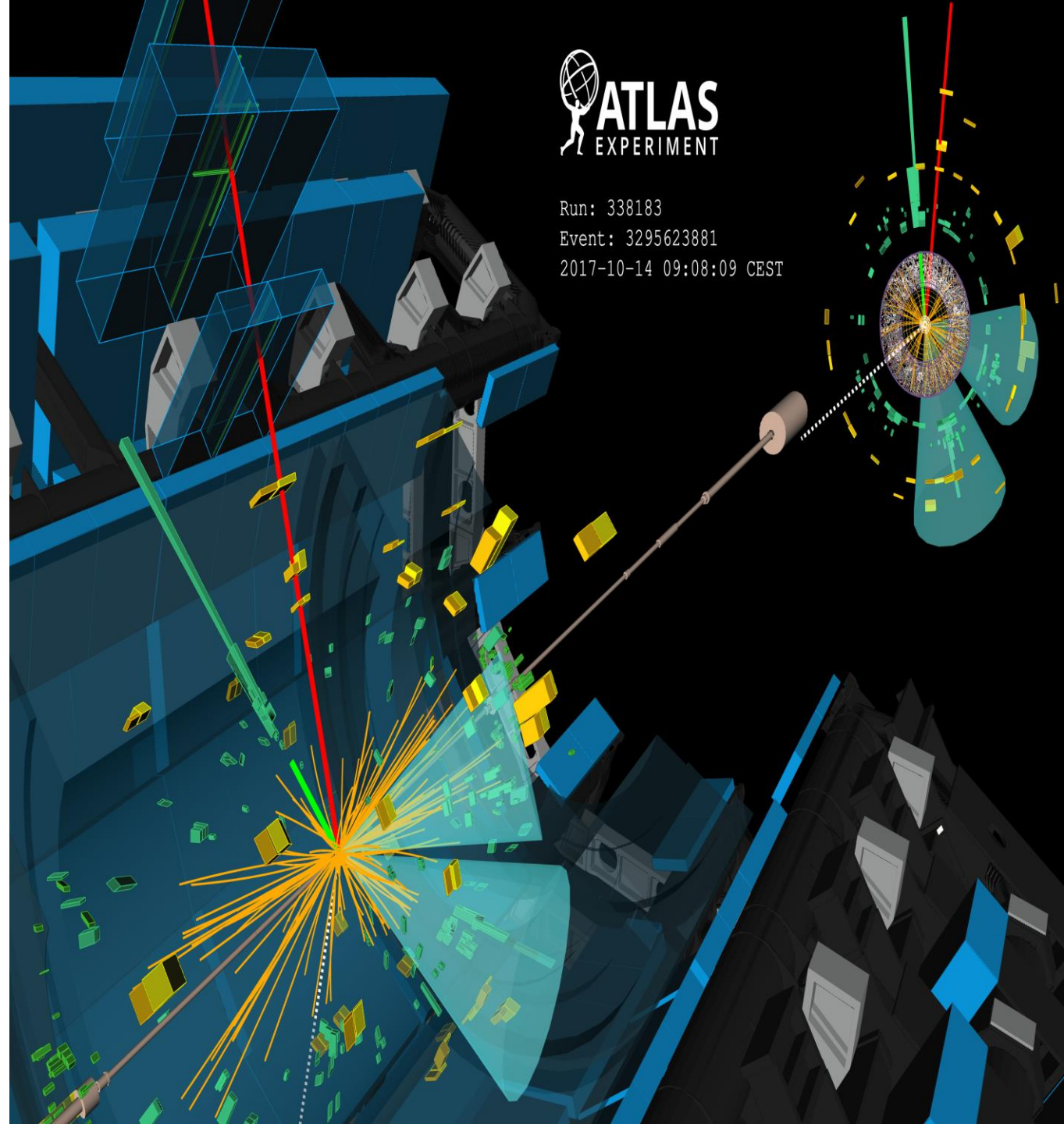


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Could this help with toponium?

Top quark

What is it?

$$m = 172.52 \text{ GeV}/c^2$$

$$q = +2/3$$

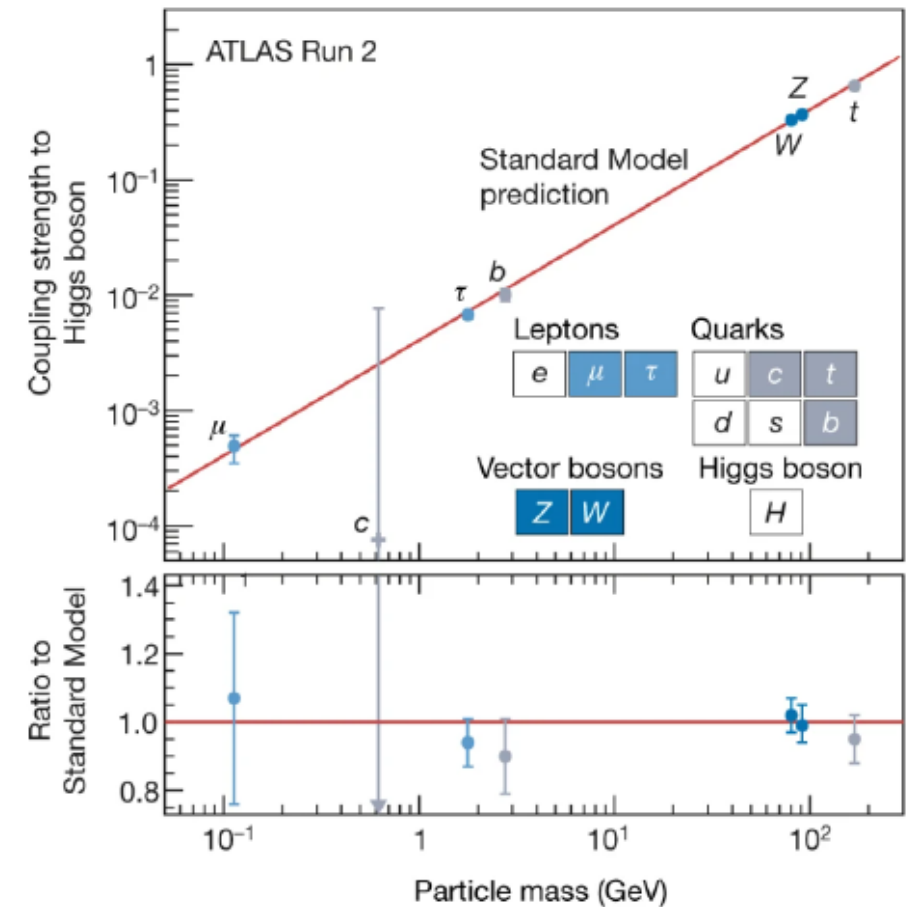
t
top

The most massive quark, 40 times more than the previous one (b quark); strongly coupled to Higgs boson

$$\tau_t \sim 10^{-25} \text{ s} < \text{hadronisation time}$$

Phys. Rev. D 110, 030001 (2024)

[Nature 6075 52-59 \(2022\)](#)



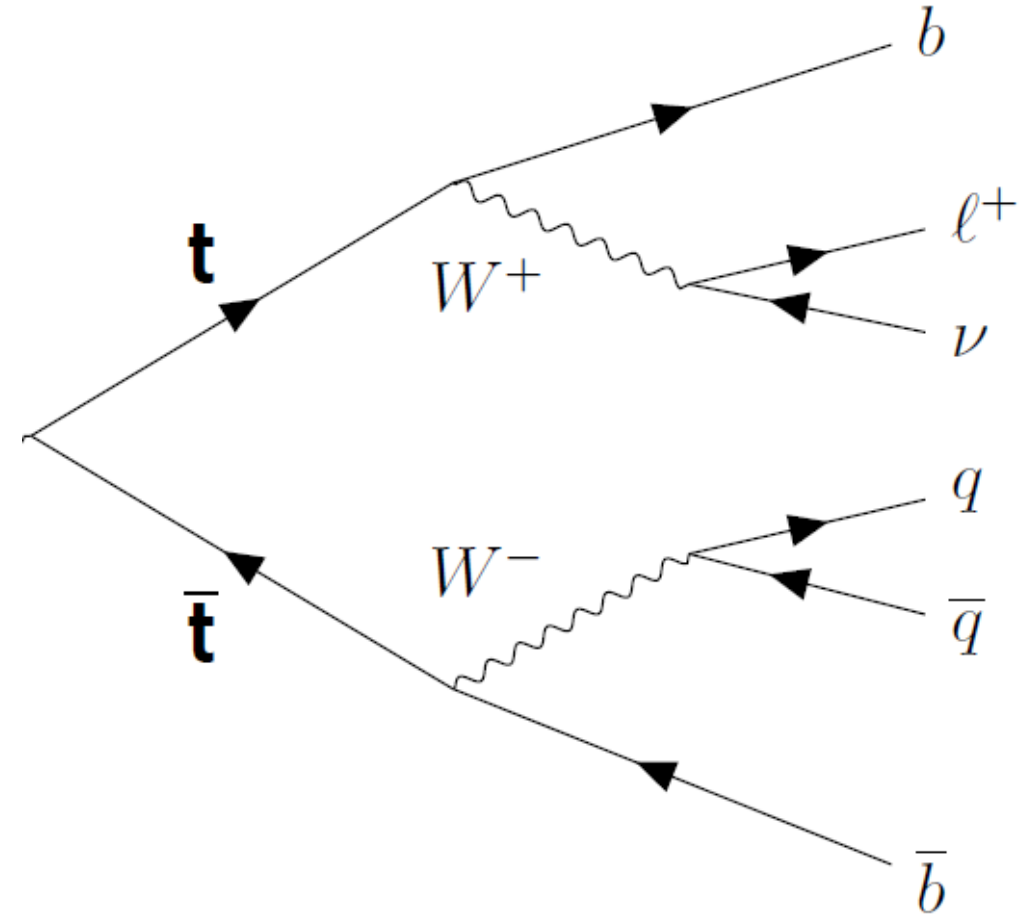
Top quark

How does the top decay?

$$\tau_t \sim 10^{-25} \text{ s} < \text{hadronisation time}$$

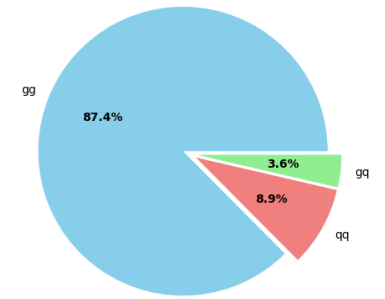
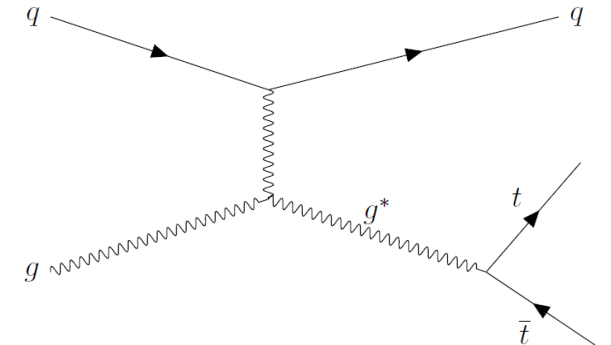
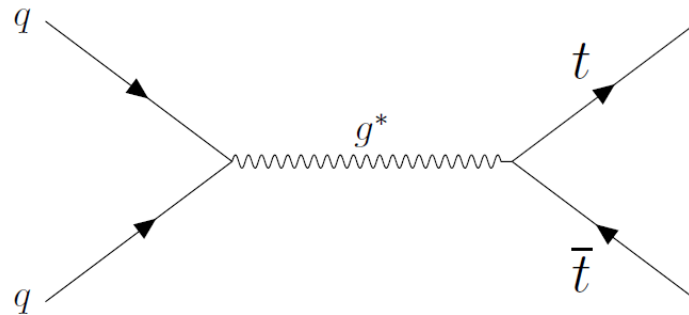
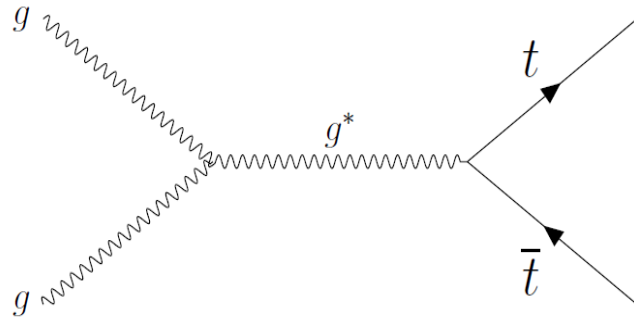
Phys. Rev. D 110, 030001 (2024)

- Semi-Leptonic (1L) decay: one W decays hadronically, the other leptonically
- Detector signature: ≥ 4 jets + MET + 1 lepton
- Leptonic t and Hadronic t



Top quark

How is top produced?



gg channel

Most abundant one

10% attractive colour singlet $^1S_0^{[1]}$

90% repulsive colour octet $^1S_0^{[8]}$

qq channel

Final state similar to gg

100% repulsive colour octet $^3S_0^{[8]}$

gq channel

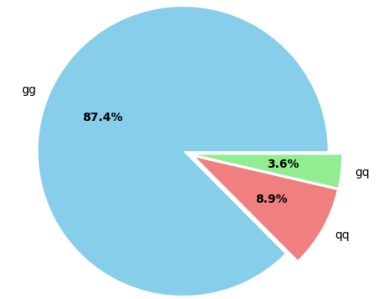
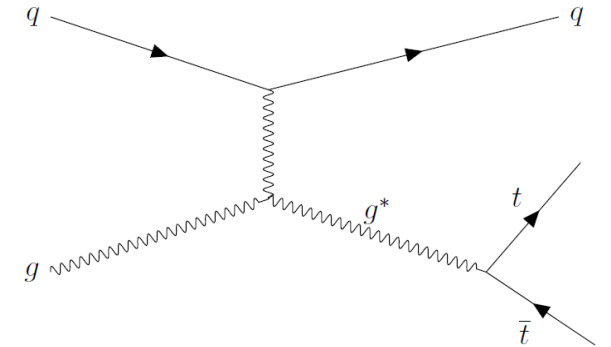
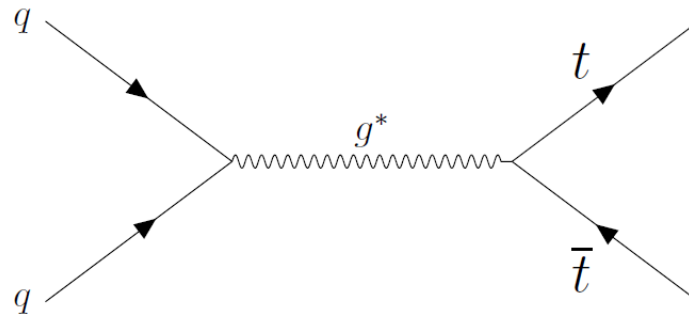
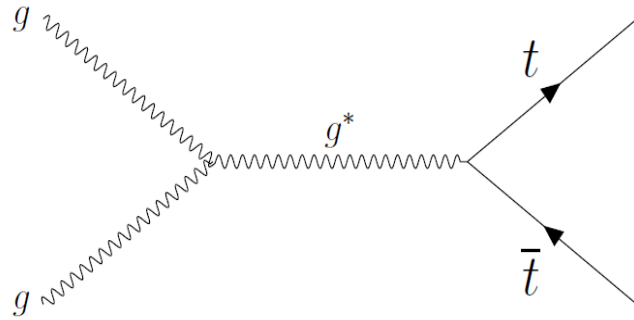
Different final state, more jets

Partially colour singlet → mixed

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Top quark

How is top produced?



gg channel

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10% attractive colour singlet $^1S_0^{[1]}$

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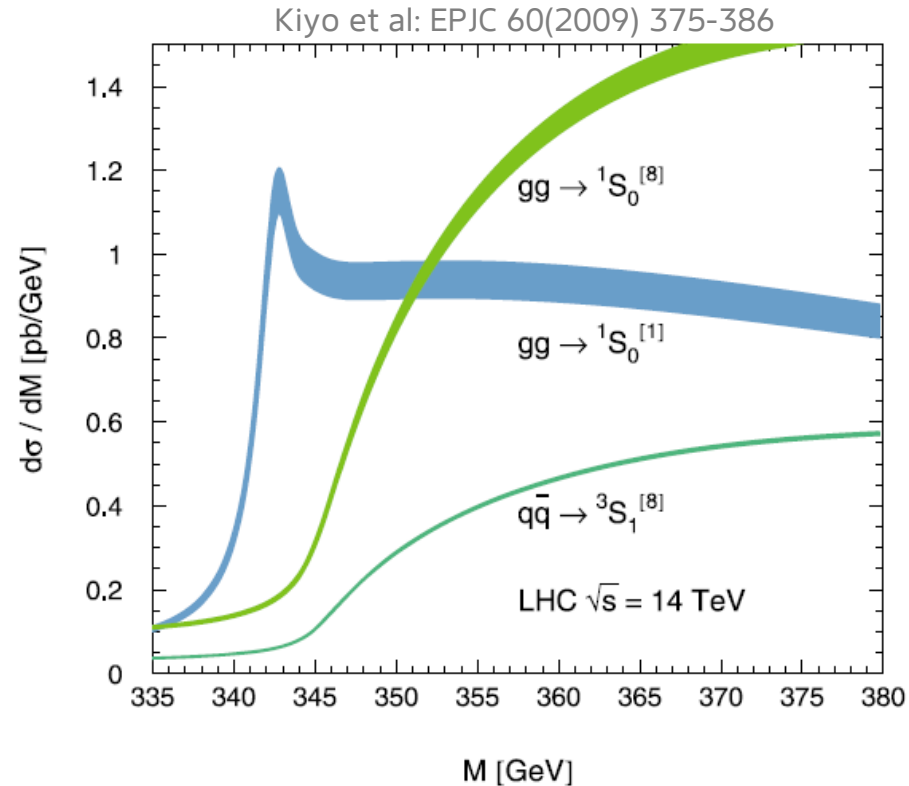
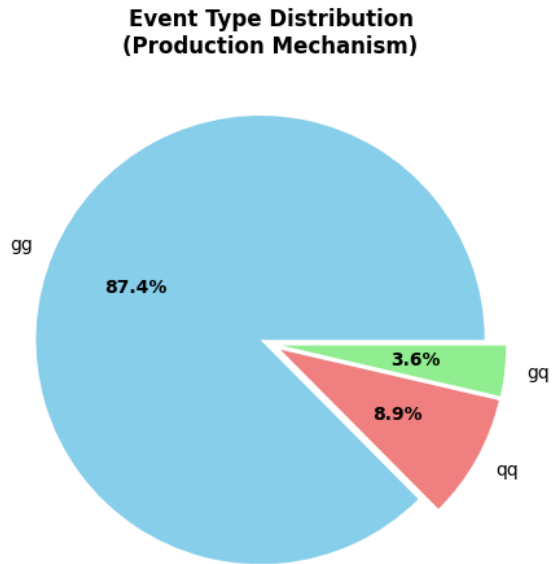
Different final state, more jets

Partially colour singlet → mixed

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Top quark

Attractive colour singlet



- Attractive colour singlet $1S_0^{[1]}$ is the good candidate for a quasi-bounded state in the threshold region
- First predicted in [1987](#) (before top observation)
- Threshold region: $M = 2 \cdot m_t$

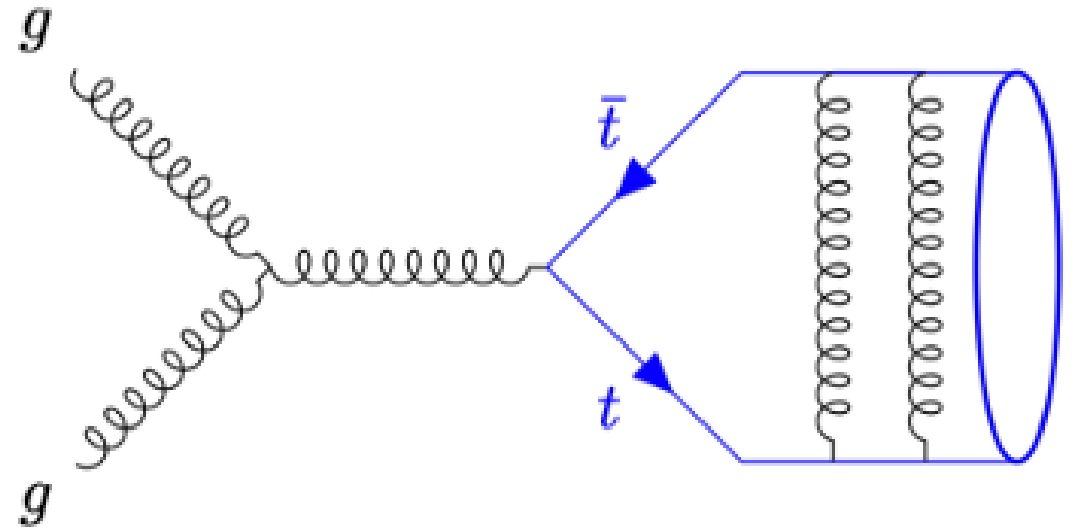
GOAL OF THIS PROJECT:

Classify the different colour states using properties of the production mode

Top quark

Quasi-bounded state

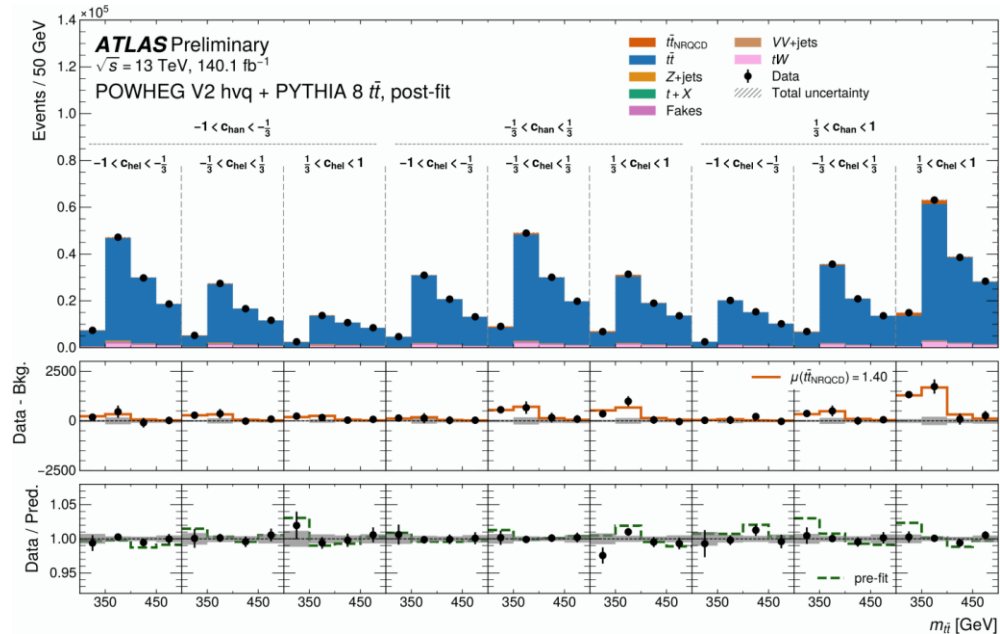
- Multiple gluon exchanges between t and $\bar{t}$
- Creation of a quasi-bounded state, called "toponium"
- Mass just below the production threshold



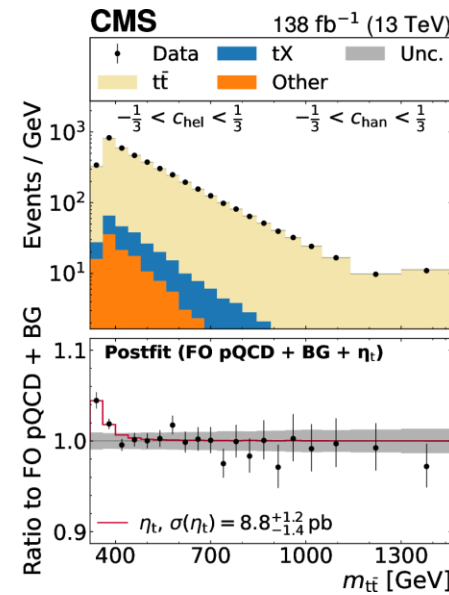
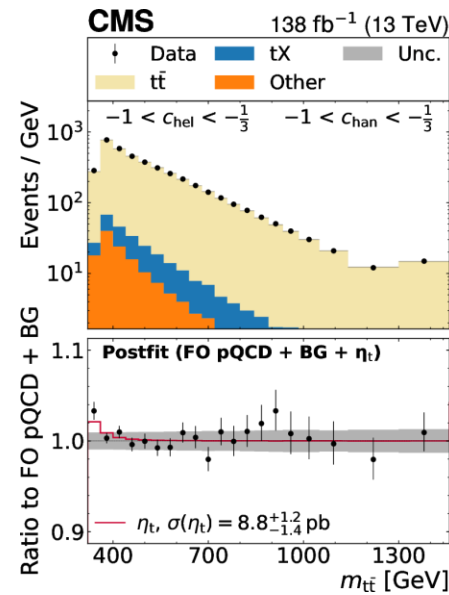
Top quark

Quasi-bounded state - observation

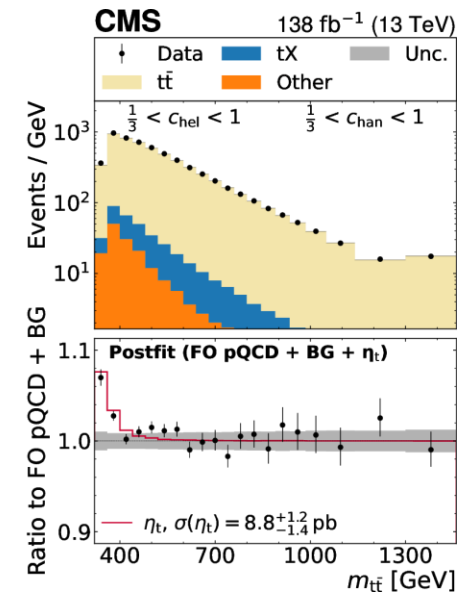
Never thought of observing it at the LHC due to low cross-section and detector resolution.
But, in 2025, it was observed, with an inclusive measurement:



[ATLAS-CONF-2025-008](#)

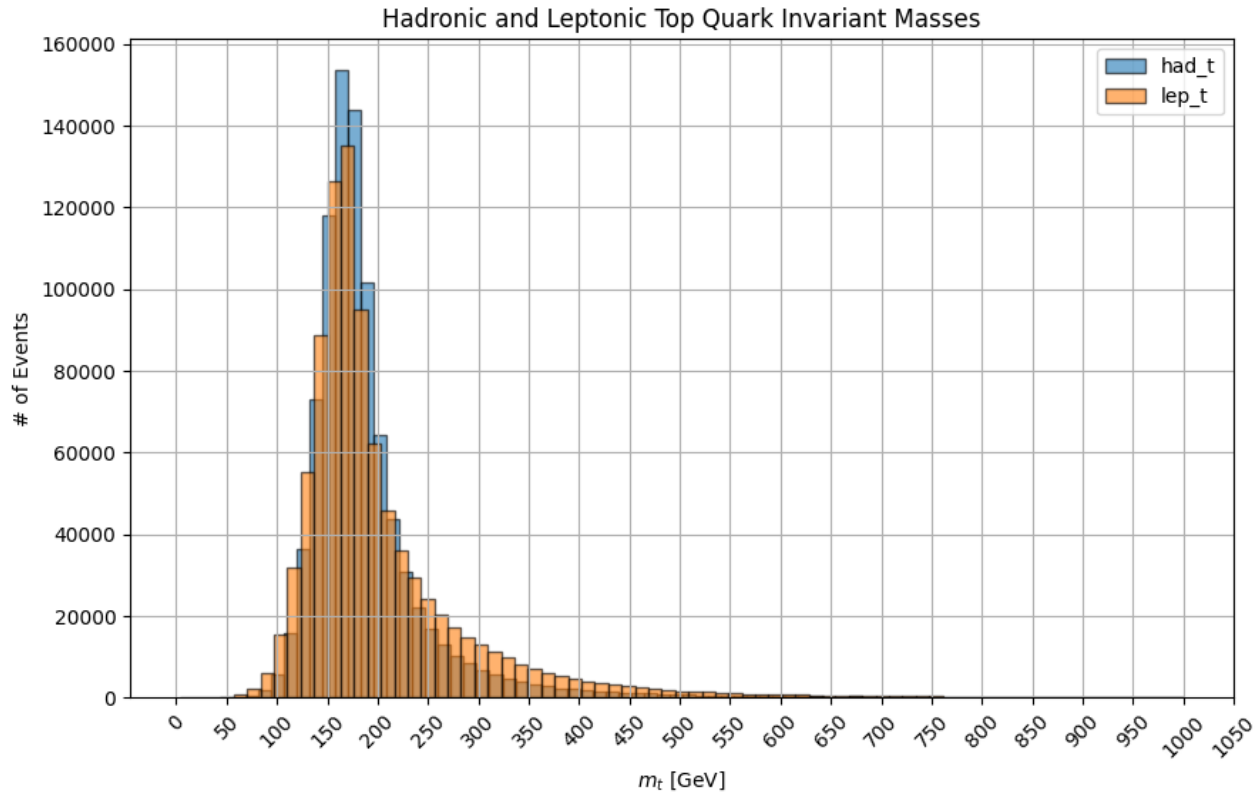


[CMS-TOP-24-007](#)



Dataset

What is our starting point?

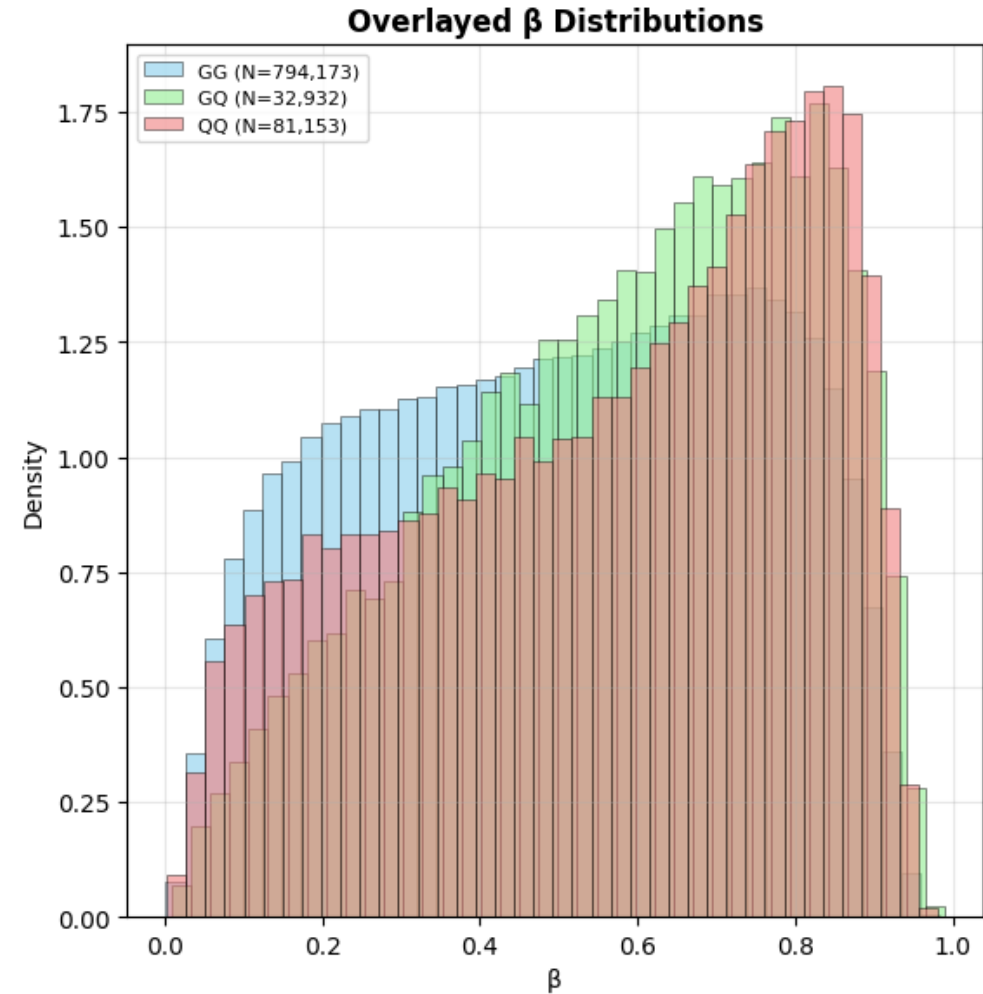


- MC simulated $t\bar{t}$ data, after $t\bar{t}$ reconstruction from SPANet
- The production channel of each event is known
- We compute four vectors of all final state particles

Dataset

Building needed bricks

- Computing high-level variables:
 - p_T for $t\bar{t}$
 - $\Delta\eta$, ΔR for $t\bar{t}$ and $b\bar{b}$
 - β
 - $|\beta_z|$
- Variables usually involved in cut-based analysis
- Good discriminating power



Dataset

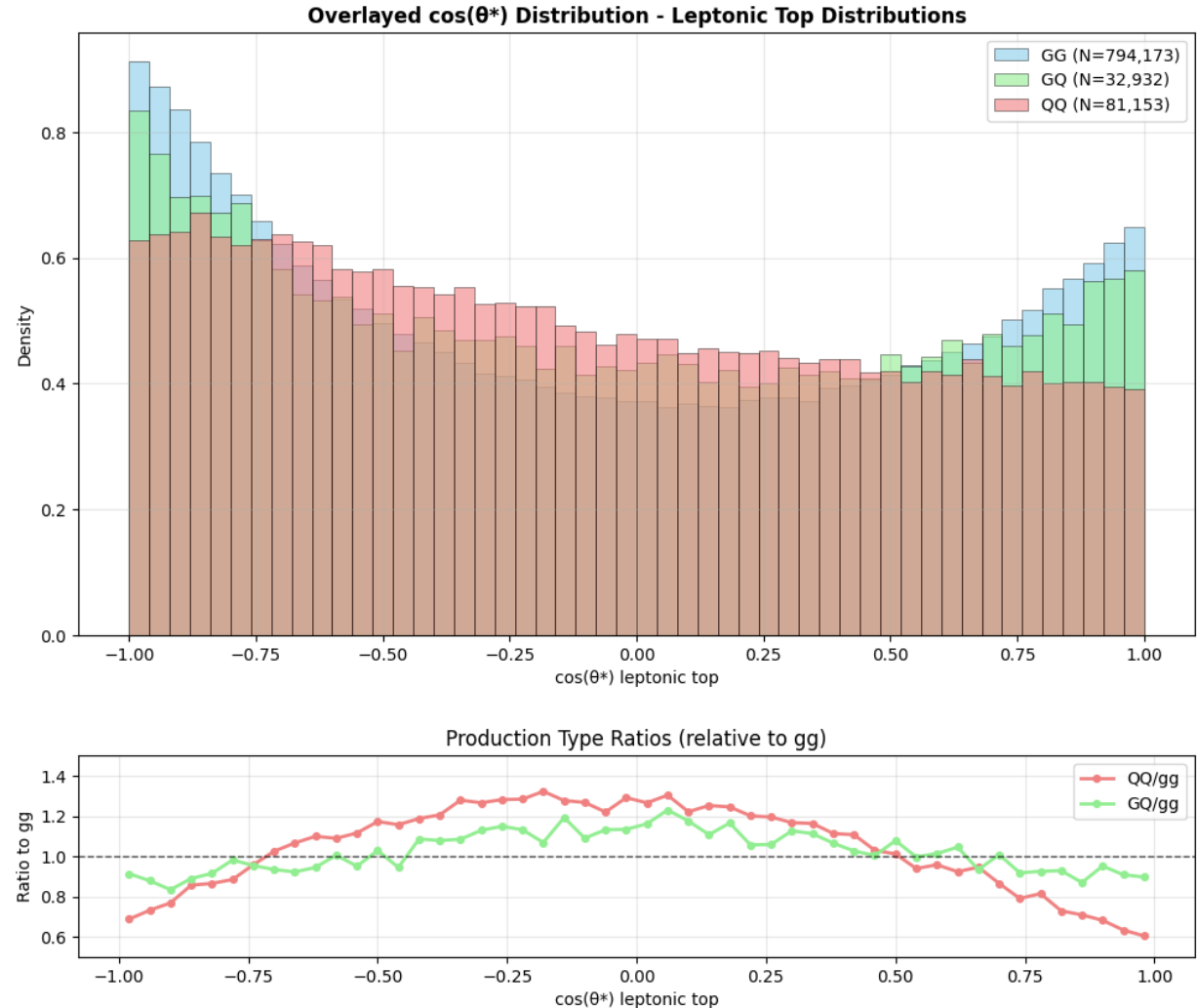
Angular variables

Also computed angular variables:

- $\cos \varphi_{ij} = \text{chel}$, angle between lepton and d-quark
- chan , same but with z flip of lepton
- $\cos \theta^*$, angle between lep/had t and flight direction of $t\bar{t}$ system

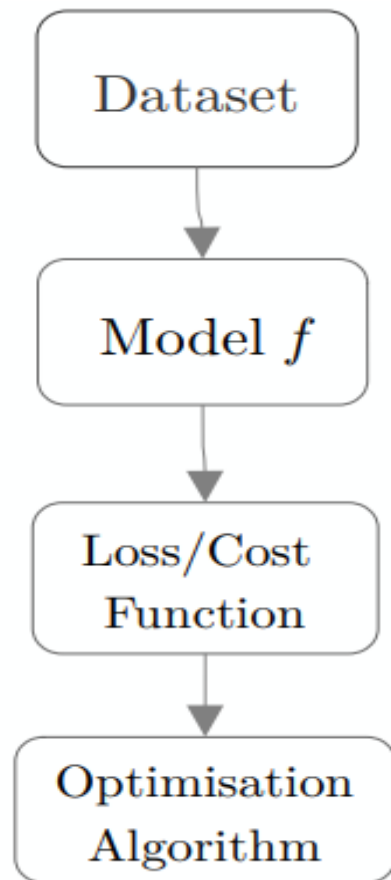
Through them, information about spin and angular distribution

$\cos(\theta^*)$ Distribution - Leptonic Top Distribution by Production Type - Overlay & Comparison



Deep Neural Network

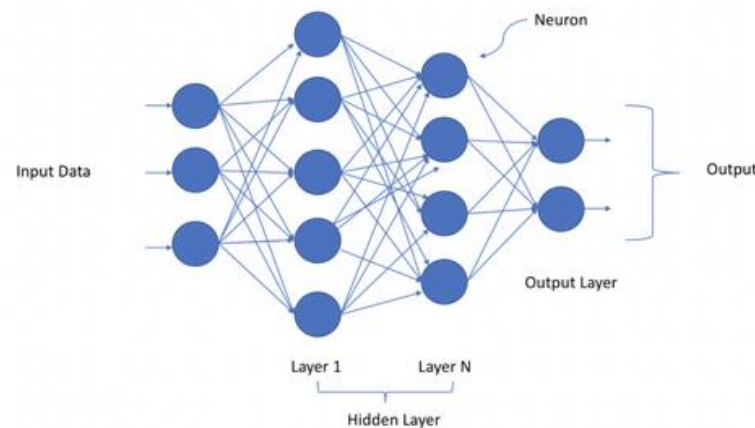
What is it?



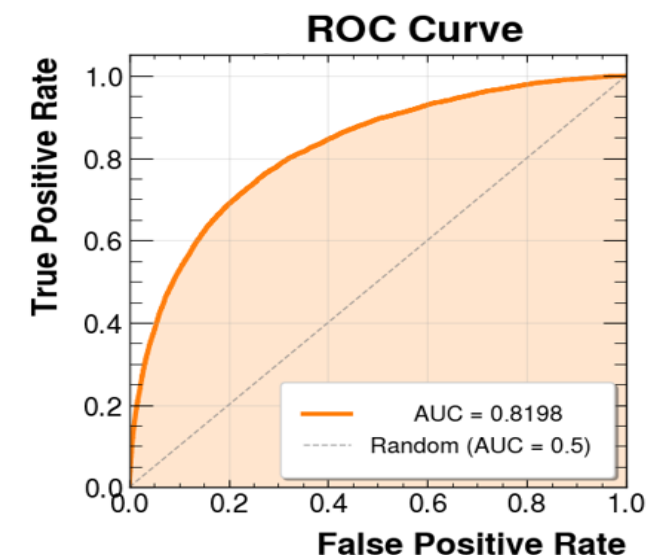
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In this study:

- **LOSS:** Binary and categorical crossentropy
- **METRIC:** weighted accuracy
- **13 FEATURES:** β , $|\beta_z|$, $m_{t\bar{t}}$, $p_{T\,t\bar{t}}$, $jets_per_event$, $\Delta\eta_{b\bar{b}}$, $\Delta R_{b\bar{b}}$, $\Delta\eta_{t\bar{t}}$, $\Delta R_{t\bar{t}}$, $\cos\varphi$, c_han , $\cos\theta_{had}$, $\cos\theta_{lep}$
- **DATASET SPLIT:**
(training, validation, testing) = (60:20:20)

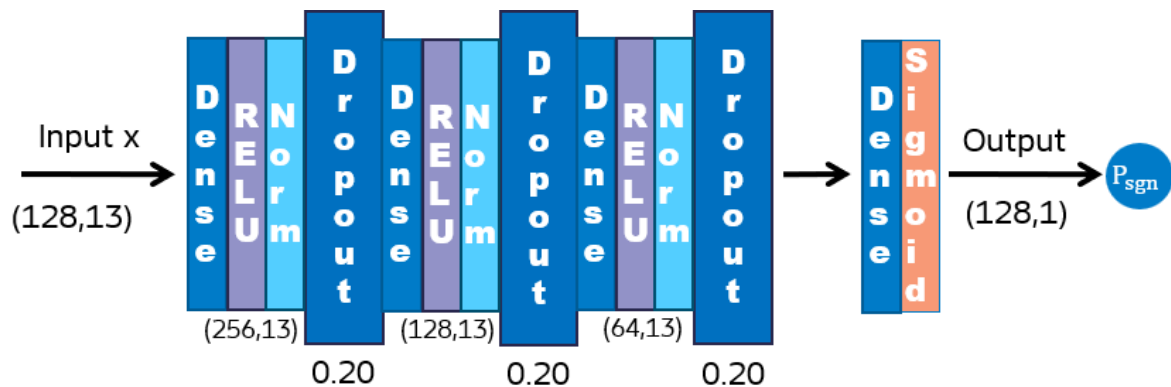


T. Lesort. Continual Learning: Tackling Catastrophic Forgetting in DNNs

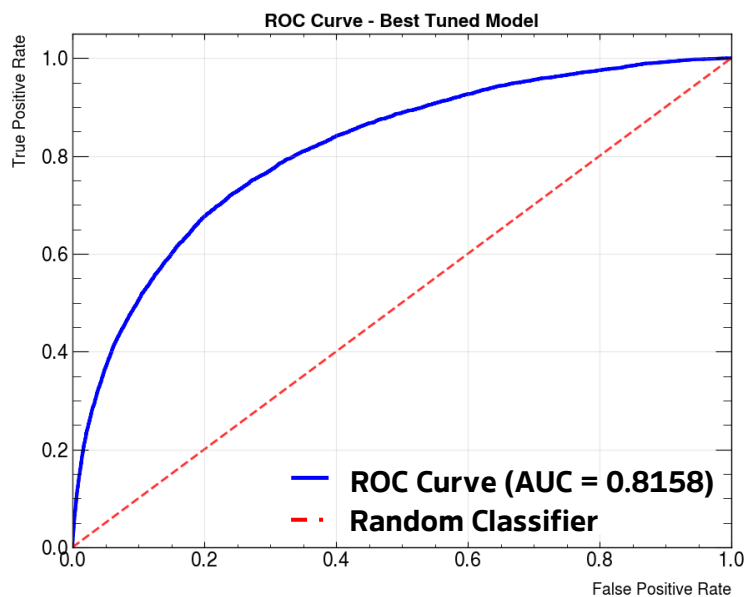
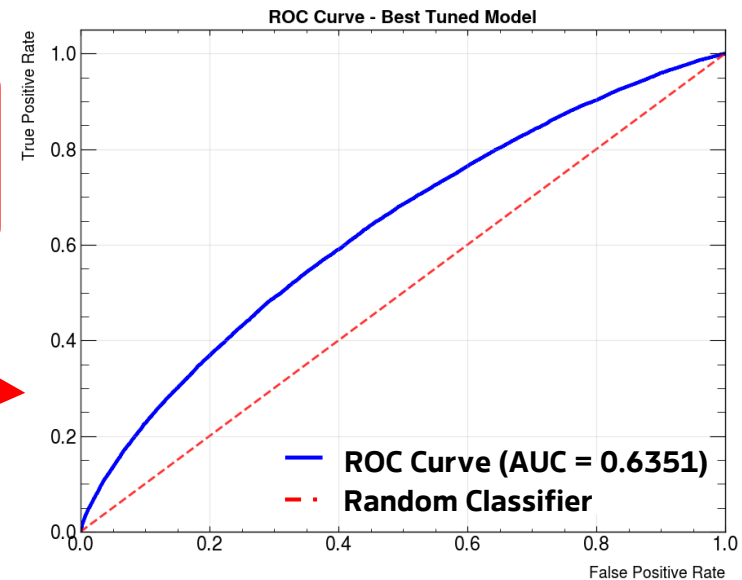


DNN implementation

Binary classification – separate analysis

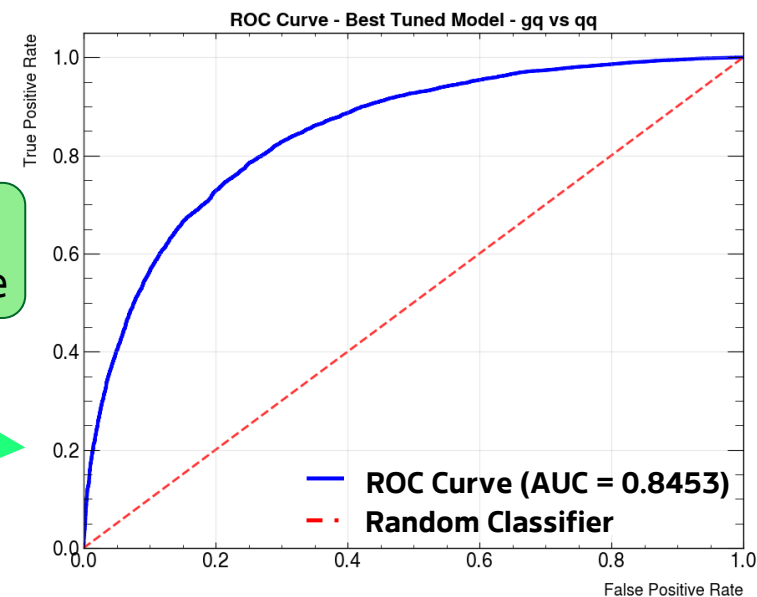


gg vs qq classifier
Not as good as
other channels!



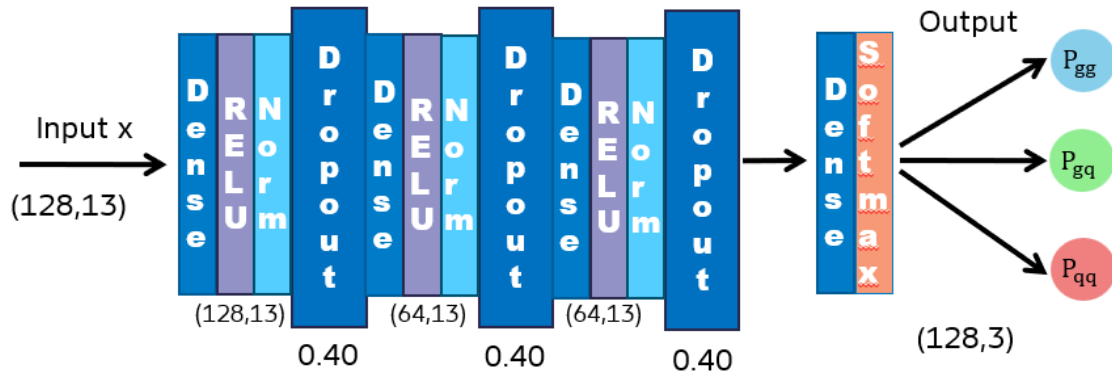
gg vs gg classifier
Good performance

qq vs qq classifier
Good performance



DNN implementation

3 classes classification – [gg,gq,qq]



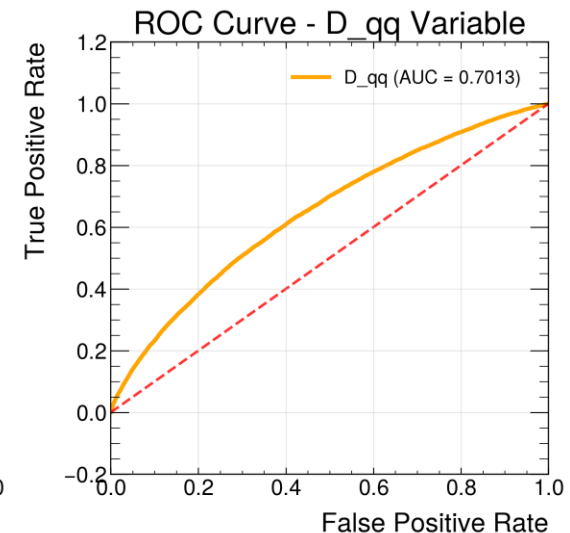
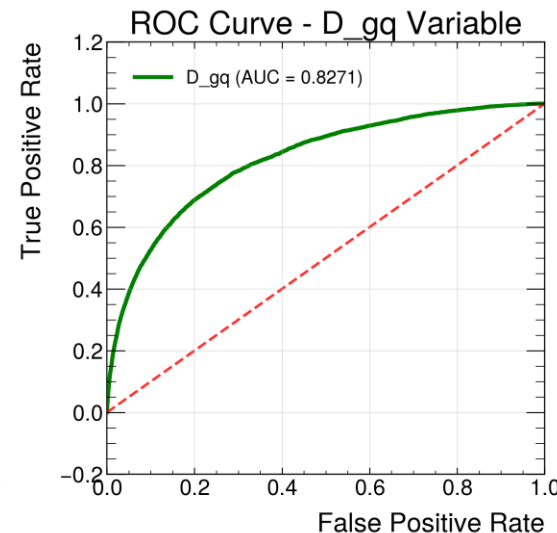
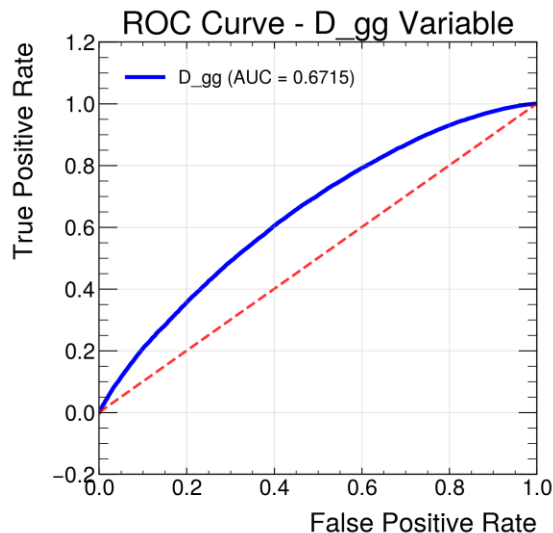
Discriminator is used to evaluate model's performance:

$$D_{gg} = \frac{P_{gg}}{f_{gq}P_{gq} + f_{qq}P_{qq}}$$

$$D_{gq} = \frac{P_{gq}}{f_{gg}P_{gg} + f_{qq}P_{qq}}$$

$$D_{qq} = \frac{P_{qq}}{f_{gg}P_{gg} + f_{gq}P_{gq}}$$

ROC Curves for D Variables (DNN Performance)



DNN implementation

Feature ranking and optimisations

- **FEATURE ANALYSIS:**

Gradient-Based Feature Importance by Tensorflow,
→ ttbar_pT most discriminant variable

- **OPTIMISATIONS:**

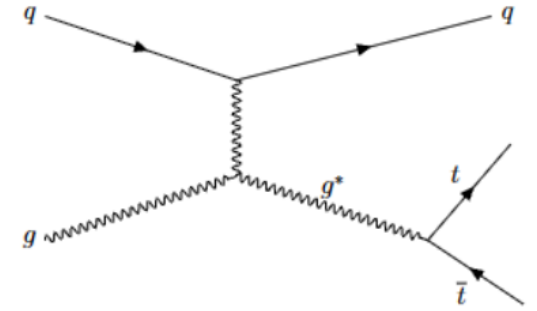
Testing different hyperparameters and choosing
the configuration with the maximum AUC

ROC Curve computed over single variables distributions: DNN is always performing better

Variable	gg vs gq	gg vs qq	gq vs qq
Beta	59.7 %	57.4 %	58.1 %
Beta_z	51.3 %	57.9 %	56.1 %
ttbar pT	77.0 %	56.5 %	53.2 %
DNN 1 node	81.6 %	63.5 %	84.5 %

Conclusions

Could this help with toponium?



- gq channel is the one we can identify better, both in the 1 node and in the 3 nodes analysis
- DNN could be more performant than classical cut-based analysis
- It is worth investigating the production modes of $t\bar{t}$ to be able to probe the threshold region more deeply: suppressing qq and gq production provides a cleaner data sample for studies of *toponium* and also other measurements, such as *quantum entanglement*
- Future outlook:
 - *Increasing statistics*: from 900K to 10M events
 - Implementing *more complex architectures* (e.g. Transformers), which would allow us to extract potential additional features and difference from low-level variables, such as the jet 4-vectors

Thank you

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ATLAS group for the hospitality*

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ATLAS
EXPERIMENT



BACKUP

Dataset

Kinematic variables computation

- Beta for ttbar system: $\beta_{t\bar{t}} = \frac{p_{t\bar{t}}}{E} \rightarrow \text{boost of the system}$
- Beta_z for ttbar system: $|\beta_{z\ t\bar{t}}| = \frac{p_{z\ t\bar{t}}}{E} \rightarrow \text{boost of the system along z-axis}$
- Delta eta: $\Delta\eta = \eta_t - \eta_{\bar{t}}$
- Delta R: $\Delta R = R_t - R_{\bar{t}}$

Dataset

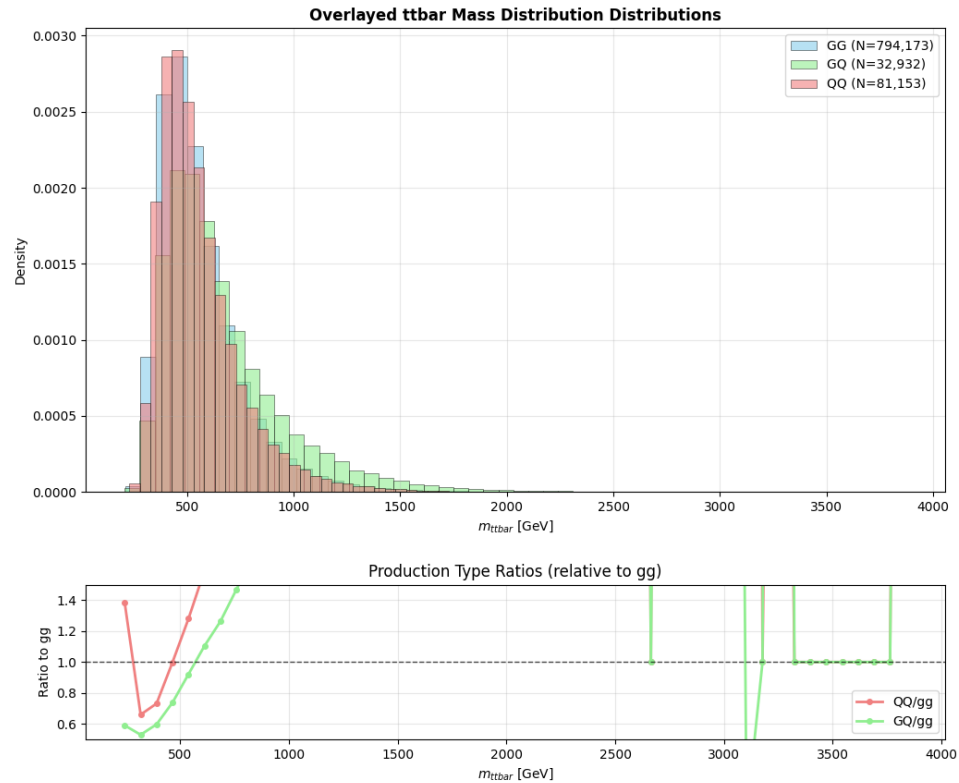
Angular variables computation

- $\cos \varphi_{ij}$ = chel : angle between lepton and down-type quark , after boosting them to top parent ref frame
 $\langle \cos \varphi \rangle = \langle \hat{\ell} \cdot \hat{d} \rangle$
- Chan: the same of $\cos \varphi$, but with flip of the z-direction of lepton before the product
- $\cos \theta^*$: angle between one top and flight direction of ttbar

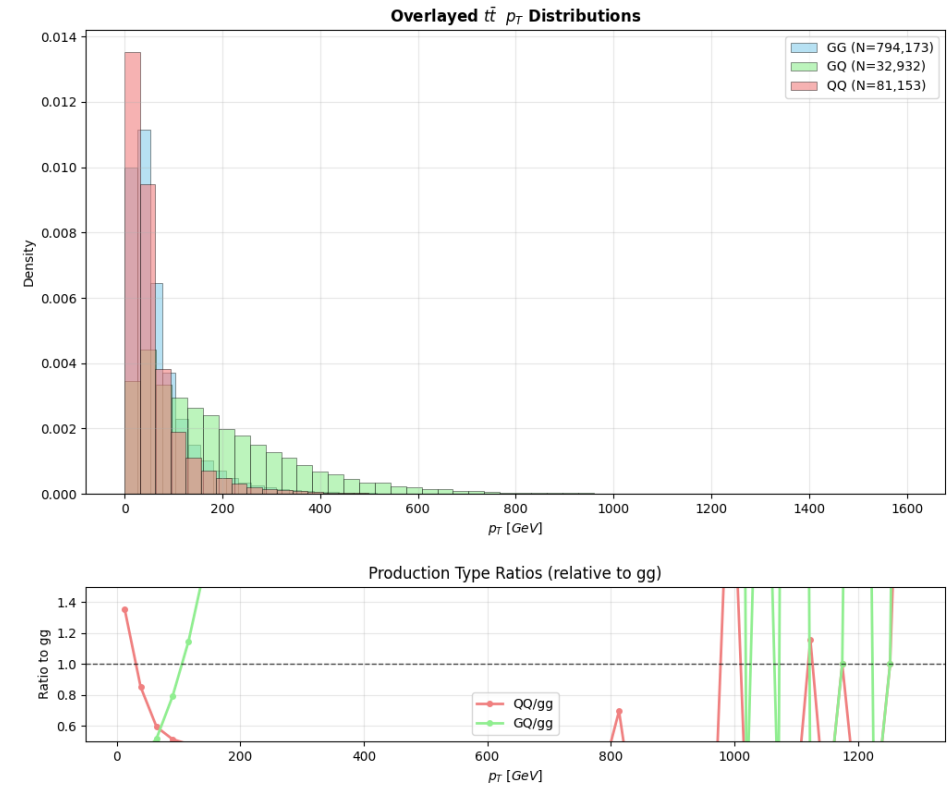
Dataset

$t\bar{t}$ invariant mass and p_T of $t\bar{t}$

$t\bar{t}$ Mass Distribution Distribution by Production Type - Overlay & Comparison

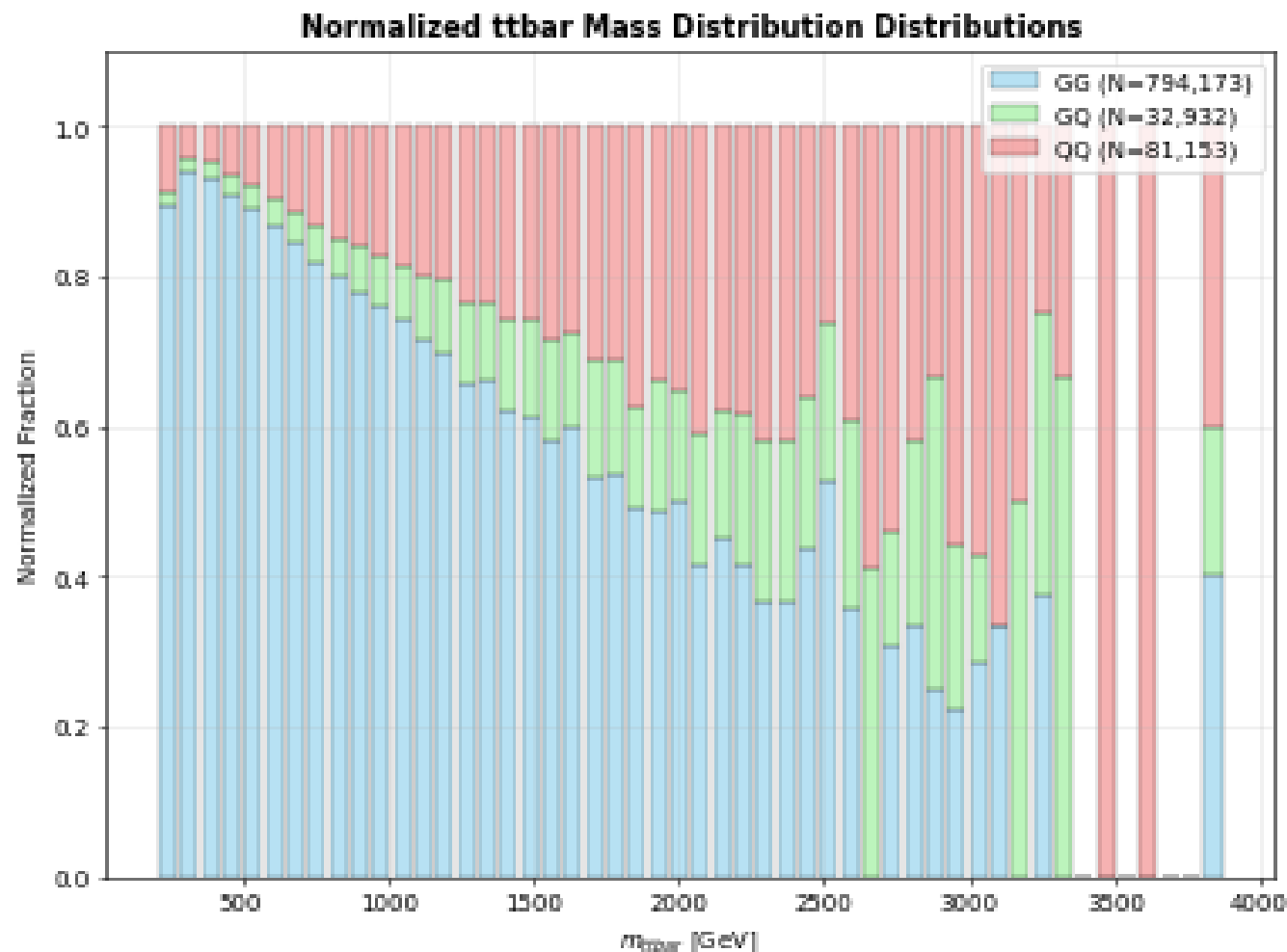


$t\bar{t}$ p_T Distribution by Production Type - Overlay & Comparison



Dataset

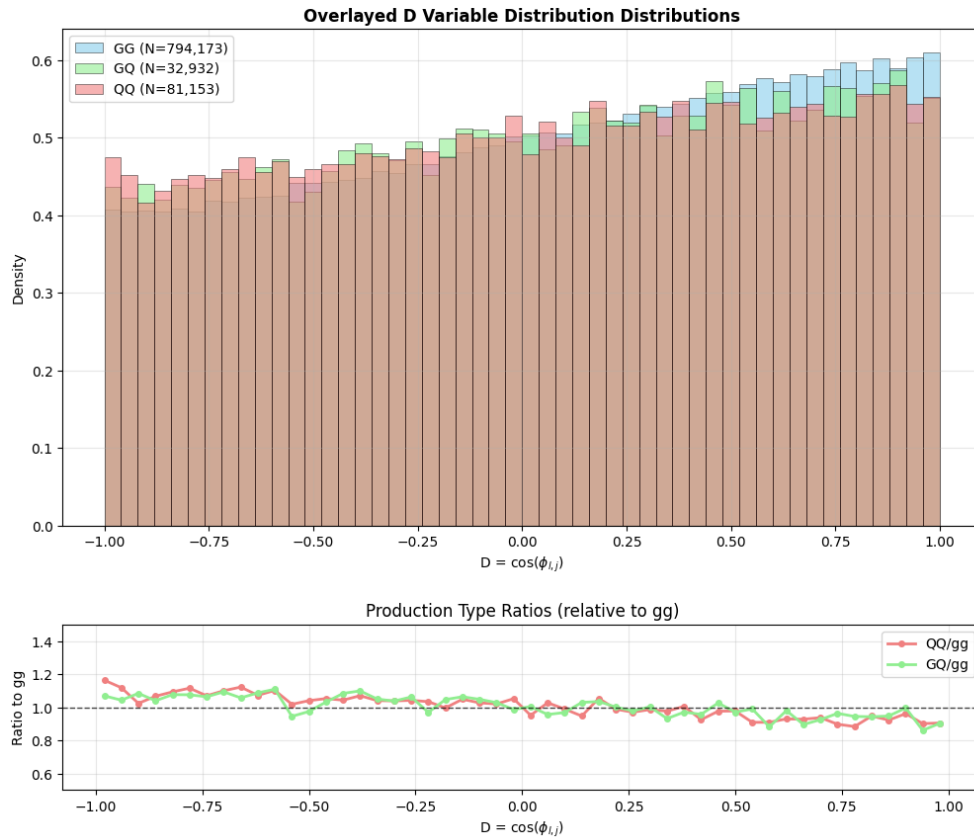
Normalized $t\bar{t}$ invariant mass per production mode



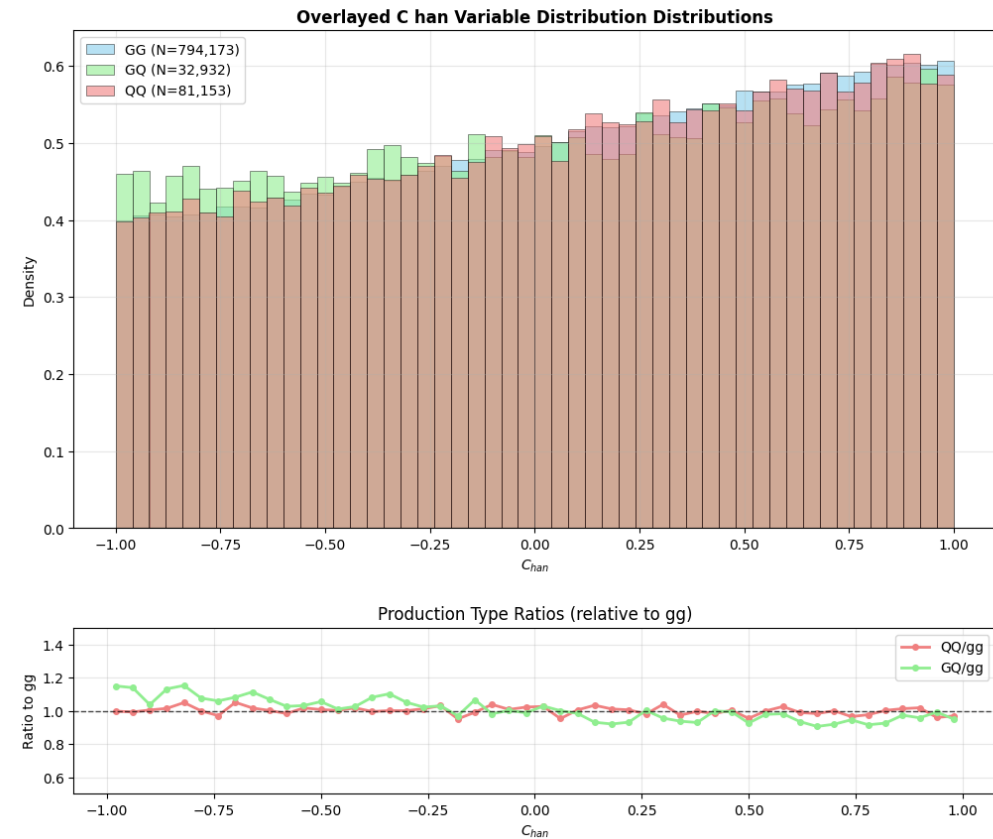
Dataset

Angular variables per production mode

D Variable Distribution Distribution by Production Type - Overlay & Comparison

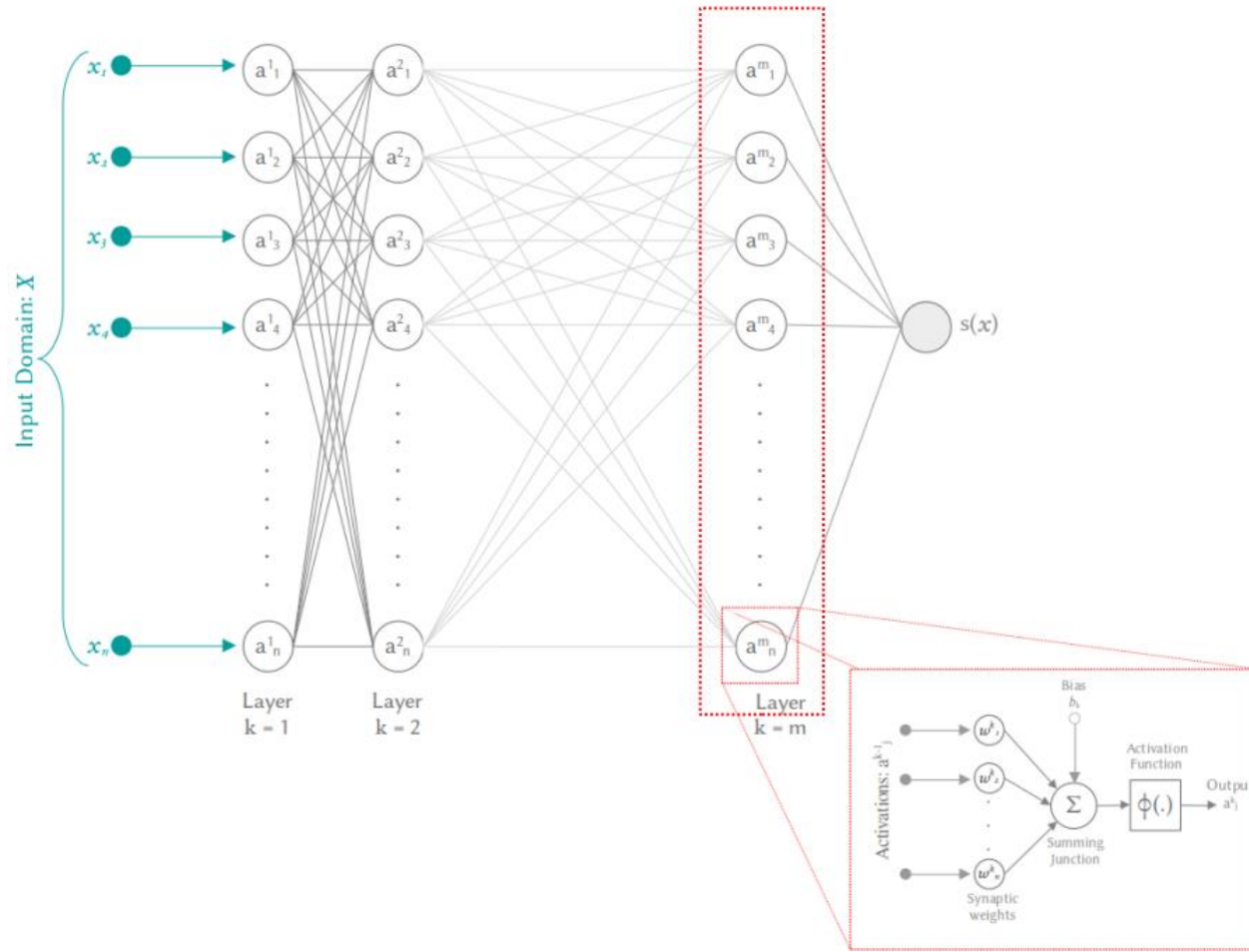


C han Variable Distribution Distribution by Production Type - Overlay & Comparison



Deep Neural Network

What is it?



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- Neuron structure:

$$a_i^{(k+1)} = \phi \left(\sum_j^n w_{i,j}^{(k)} a_j^{(k)} + b^{(k)} \right)$$

- Neural Network:

$$\begin{bmatrix} a_0^{(k+1)} \\ \dots \\ a_n^{(k+1)} \end{bmatrix} = \phi \left(\begin{bmatrix} w_0^{(0)} & \dots & w_n^{(0)} \\ \dots & \dots & \dots \\ w_0^{(k)} & \dots & w_n^{(k)} \end{bmatrix} \begin{bmatrix} a_0^{(k)} \\ \dots \\ a_n^{(k)} \end{bmatrix} + \begin{bmatrix} b_0^{(k)} \\ \dots \\ b_n^{(k)} \end{bmatrix} \right)$$

Binary and categorical crossentropy loss

- Binary crossentropy (BCE):

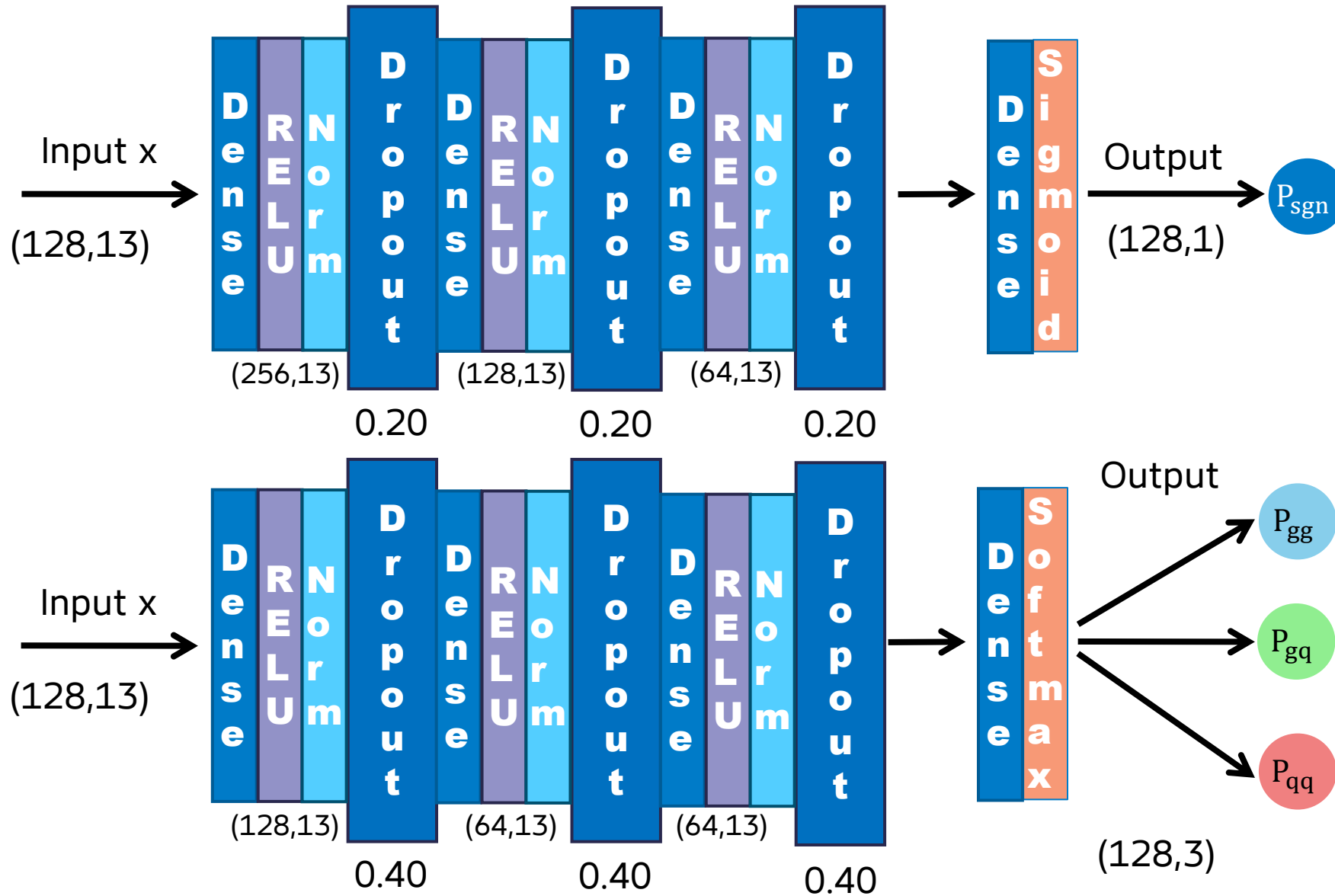
$$\text{BCE} = -\frac{1}{N} \sum_{i=1}^N [y_i \log(p_i) + (1 - y_i) \log(1 - p_i)]$$

Binary Cross-Entropy measures the distance between the true labels and the predicted probabilities. When the predicted probability p_i is close to the actual label y_i , the BCE value is low, indicating a good prediction.

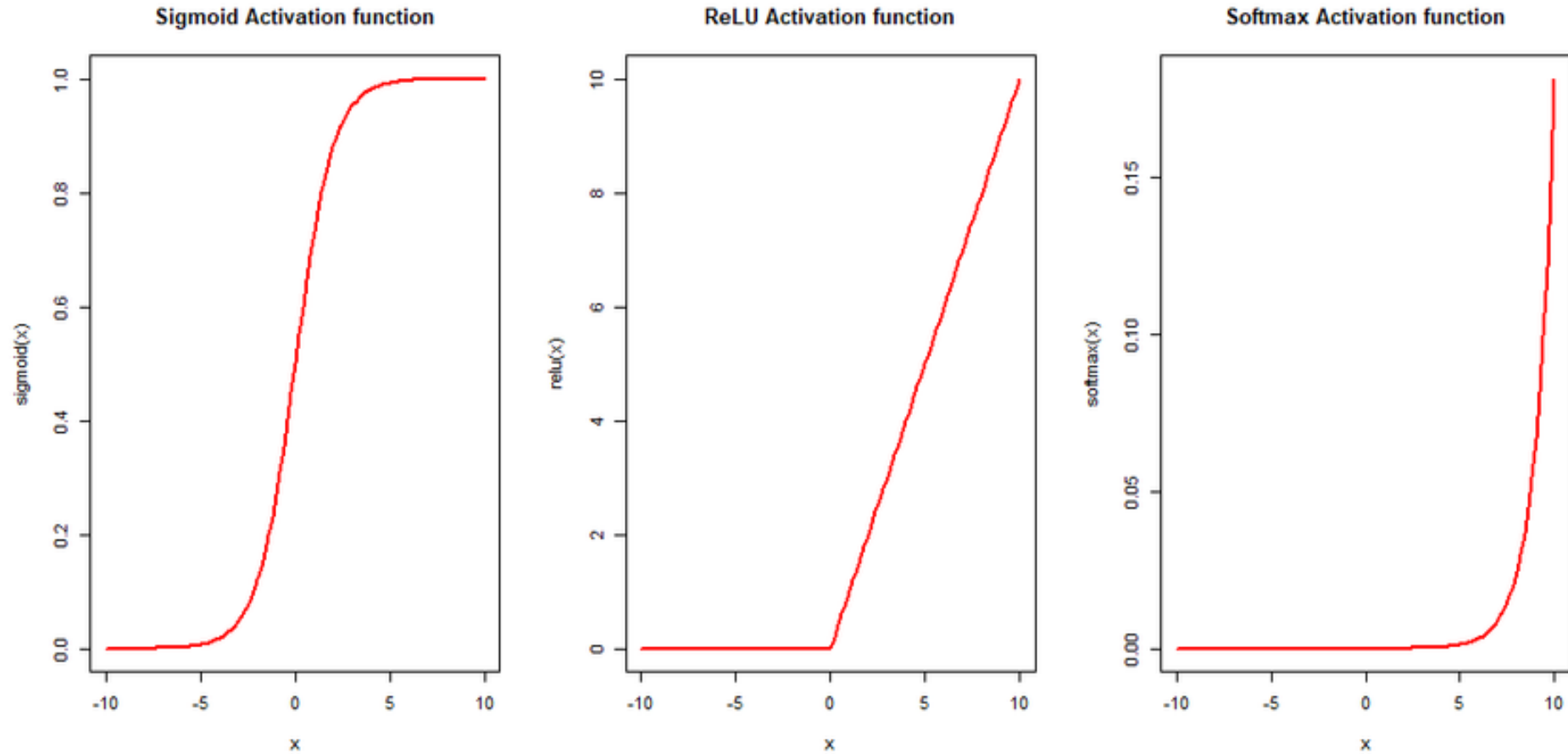
- Categorical crossentropy

$$L(y, \hat{y}) = - \sum_{i=1}^C y_i \log(\hat{y}_i)$$

Model architecture



Different activations



DNN implementation

Consistency checks

- BDT training to cross-check results
- ROC curve and AUC score over most important variables' distribution (Beta, Beta_z, ttbar pT)
- Run without angular variables → no major changes

BDT confirms results from DNN

Classical AUC	gg vs gg	gg vs qq	qq vs qq
BDT	80.9 %	83.8 %	63.7 %
Beta	59.7 %	57.4 %	58.1 %
Beta_z	51.3 %	57.9 %	56.1 %
ttbar pT	77.0 %	56.5 %	53.2 %

Discriminator AUC	gg signal	qq signal	qq signal
BDT 3 classes	64.3 %	81.9 %	64.5 %

BDT documentation

DNN is performing better

Features ranking – BDT (gg vs qq channel)

