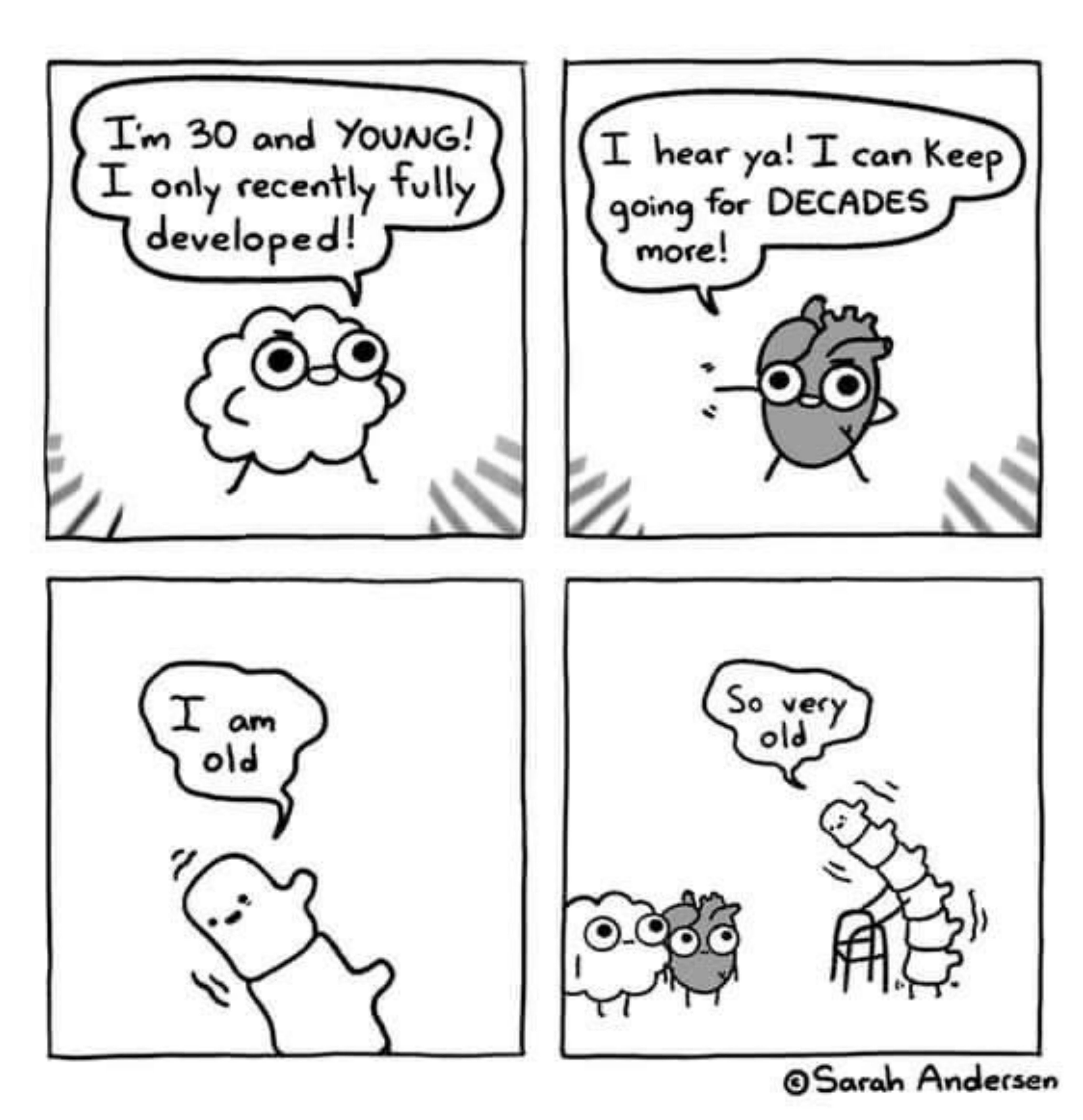
Multi-scale Cross-Attention Transformer encoder for event classification

Mihoko Nojiri(IPNS, KEK), with Ahmed Hammad and Stefano Moretti
arXiv 2401.00452

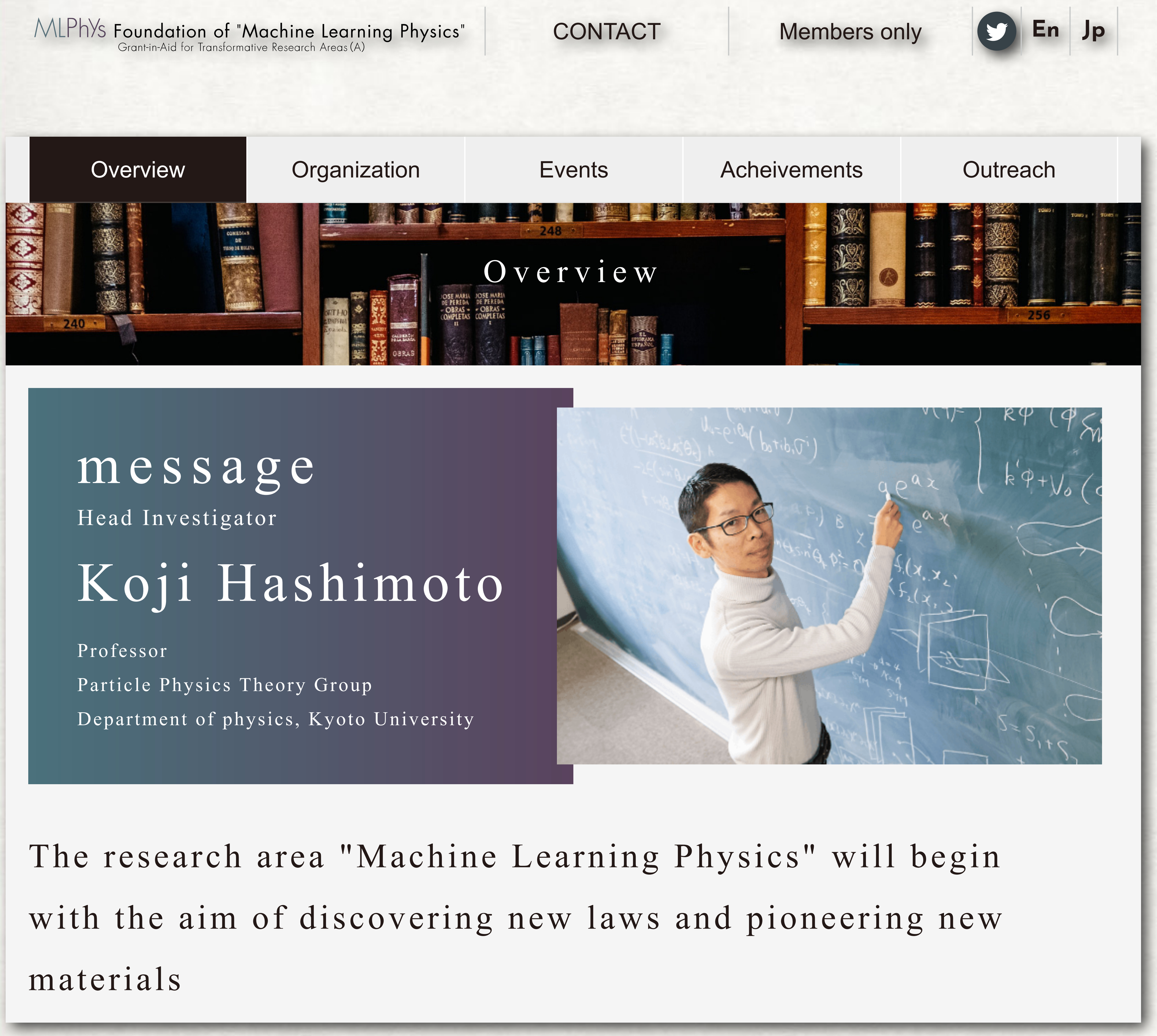
ABOUT MYSELF

"a young mind",
(according to Tilman Plehn)
but this makes me cry

- PhD Kyoto (1990) a bit old(61)
- PD: Supergravitiy study in heavy top era →   SUSY dark matter. Sommerfeld effect in dark matter annihilation. (2003)
- Collider phenomenology:
  - 1996: JLC study: Meeting LHC people in Snowmass in USA
  - 2002-2008 LHC BSM study in ATLAS SUSY group. BSM Convener of Les Houches TeV collider workshop twice (2003, 2007) → Jet substructure study → **Deep Learning**
- **Service**: JPS executive board member →member of Science Council of Japan(SCJ) [2017-2023] working on Gender Diversity Issues .
  - In KEK, DEI workshop Dec 2023 (https://www2.kek.jp/ipns/en/news/5320/) , trying establish DEI task force



ML(THEORY) IN JAPAN: GRANT "MACHINE LEARNING PHYSICS"

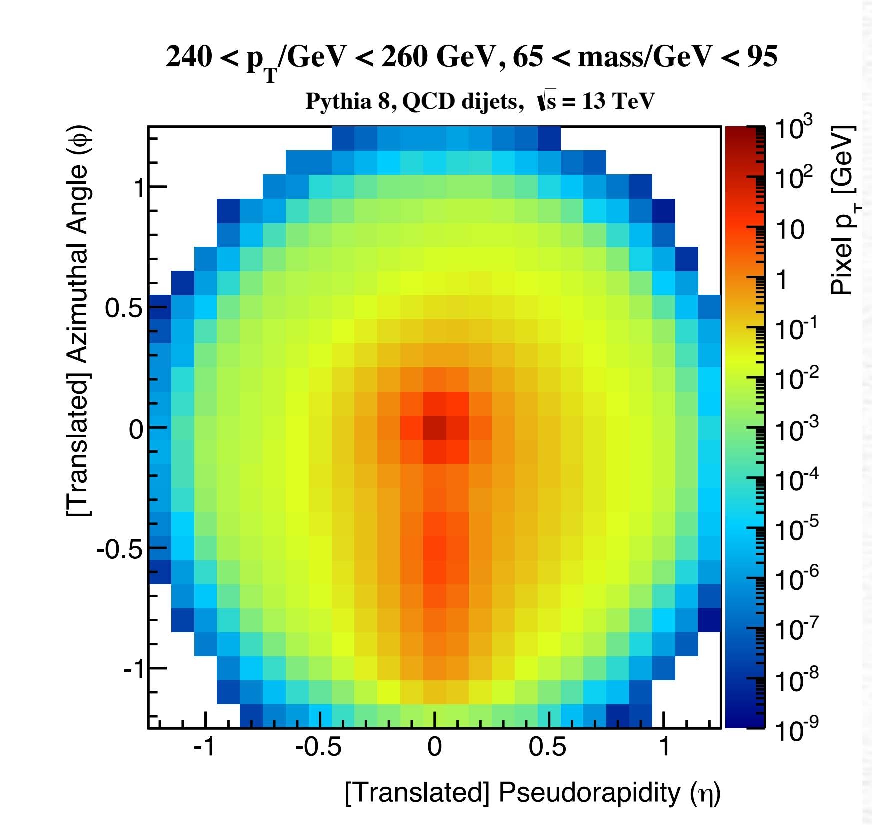


B01 Akinori Tanaka (Riken AIP) Math and application of DL
B02 Yoshiyuki Kabashima (Tokyo) Statistical data and ML
B03 Kenji Fukushima (Tokyo) Topology and Geometry of ML
A01 Akio tomiya (IPUT Osaka) Lattice
A02 Mihoko Nojiri HEP
Junichi Tanaka (ICEPP Tokyo, ATLAS)
Masako Iawasaki (Osaka Metropolitan Belle II)
Noriko Takemura and Hajime Nagahara (Data Science)
A03 Tomi Ohtsuki (Sophia U) Condensed Matter
A04 Koji Hashimoto Quantum and Gravity

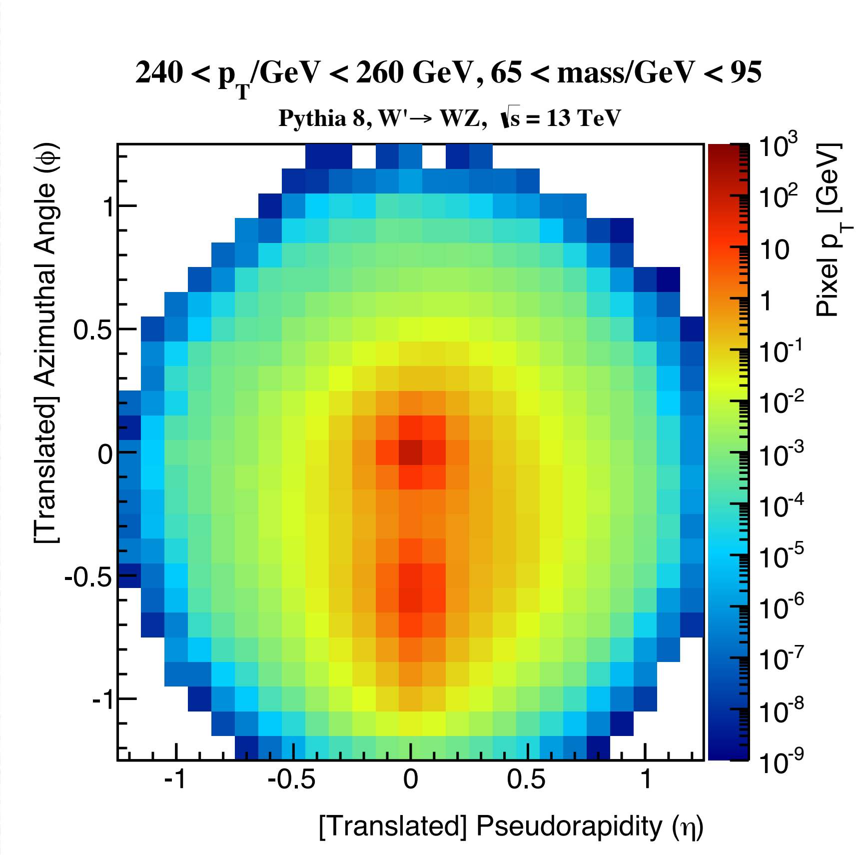
Ahmed Hammad
2017-2020: Ph.D Basel University, Basel Switzerland
2020-2023: SeoulTech, Korea
2023- KEK

Jet classification using ML

QCD jet
(in W mass region)



W jet



from Schwartzman et all
https://iopscience.iop.org/article/10.1088/1742-6596/762/1/012035

Motivation

SM Higgs sector : metastability →New Physics

DM, neutrino → New Physics

Weaker constraint for third generation fermions and Higgs.

Experimental situation

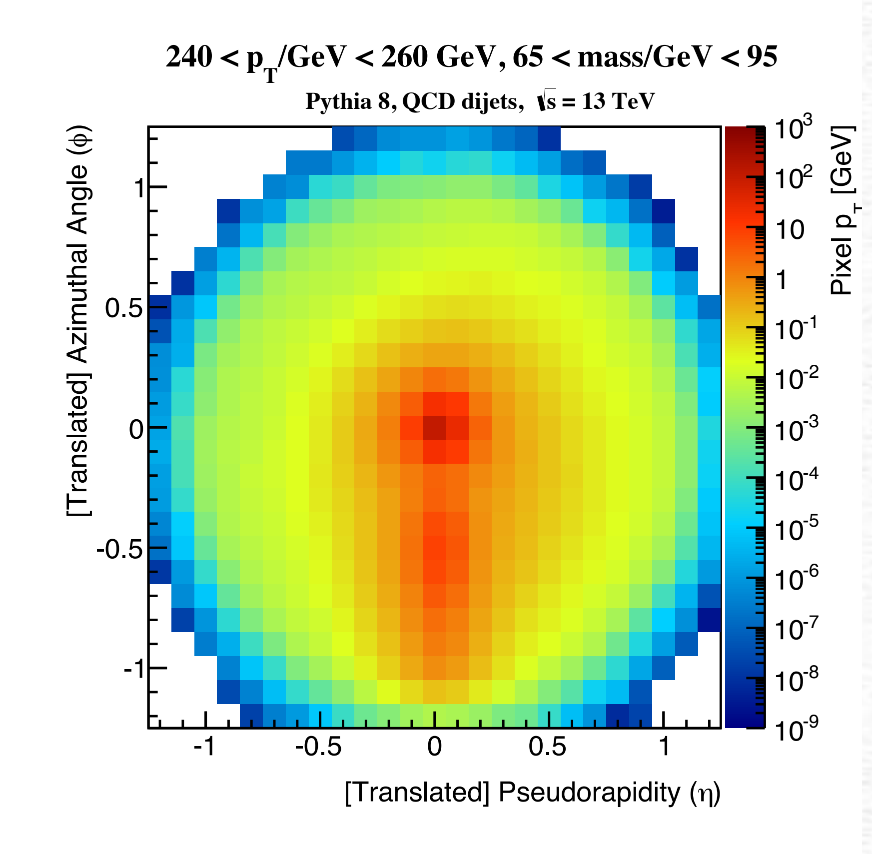
High Luminosity often dominated by background

→ need Higher Rejection of background.

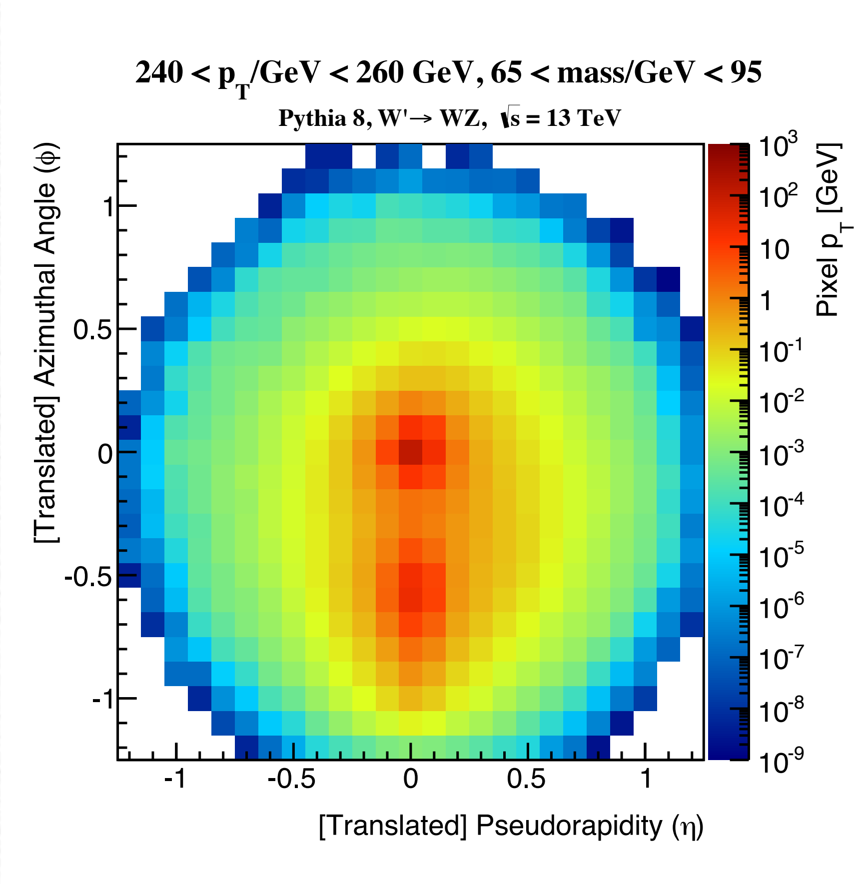
Sensitivity under S/BG~1 scale by $1/\sqrt{N}$ → background rejection $1/N$

Jet classification using ML

QCD jet
(in W mass region)

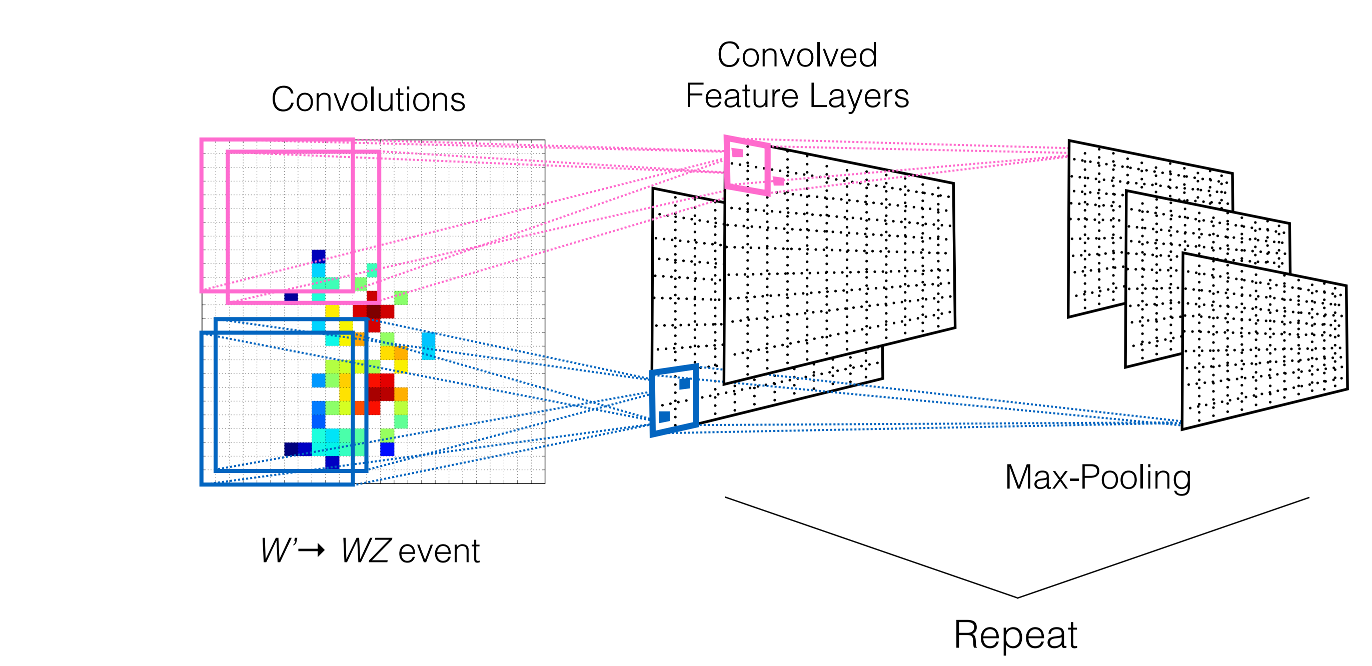


W jet



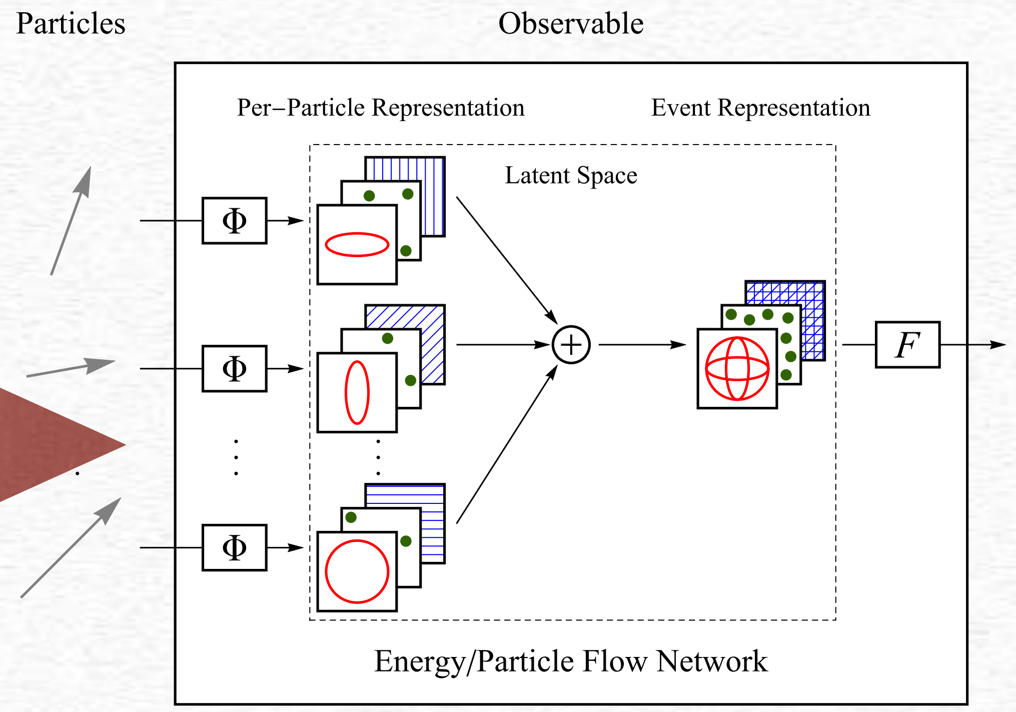
from Schwartzman et all
https://iopscience.iop.org/article/10.1088/1742-6596/762/1/012035

Jet Image



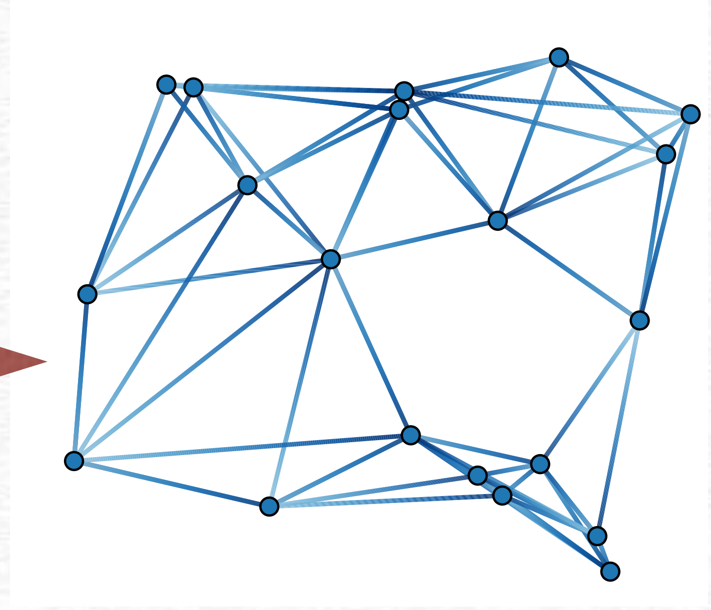
CNN Oliverira et al
(1511.05190)

as sets



permutation invariance
(Energy Flow Network and
Particle Flow Network 1810.05165)

as graphs



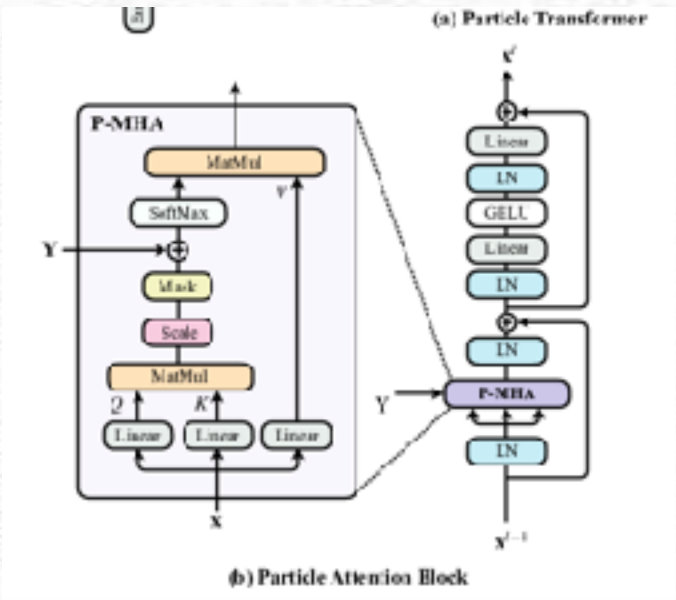
sparse data

1902.08570 Particle Net

Dreyer et al LundNet (1807.04758)

Gong et al LorentzNet(2201.08187)

transformer



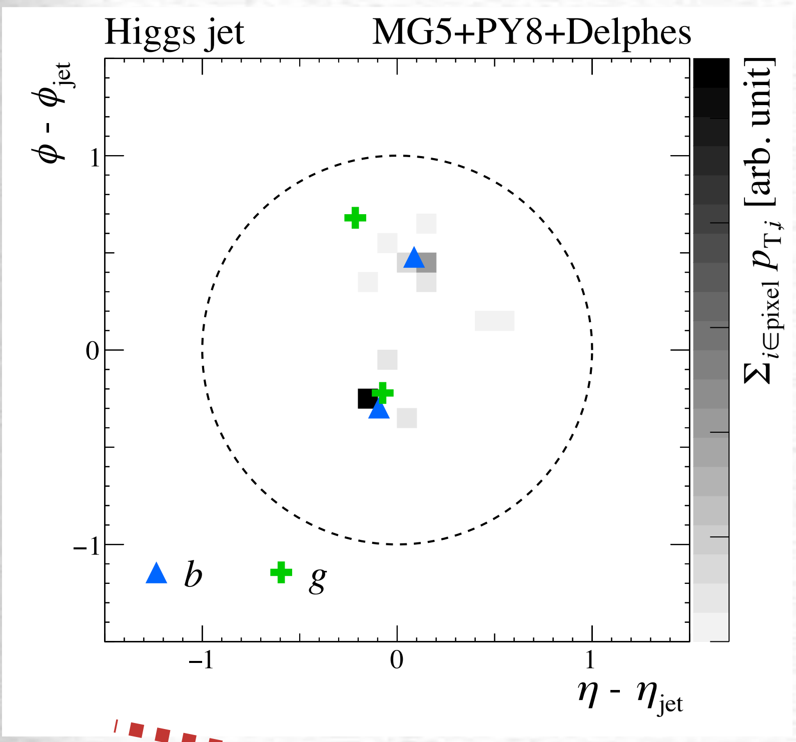
building key
and query
2202.03772

Bogatskiy et al PELICAN (2211.00454)

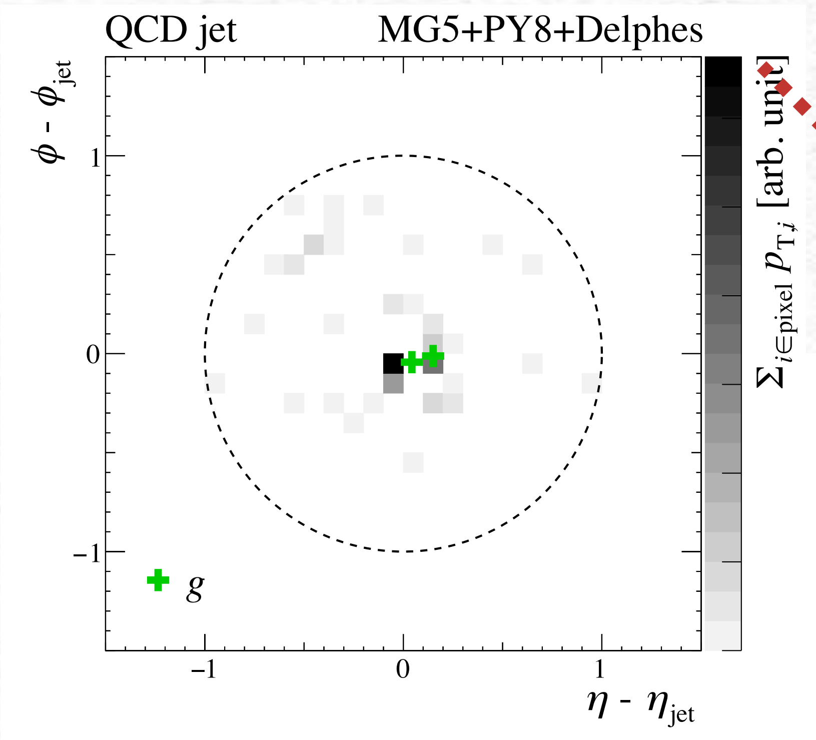
MLP :fundamental building block of ML

Input:Jet images

Higgs h+Z(→νν)



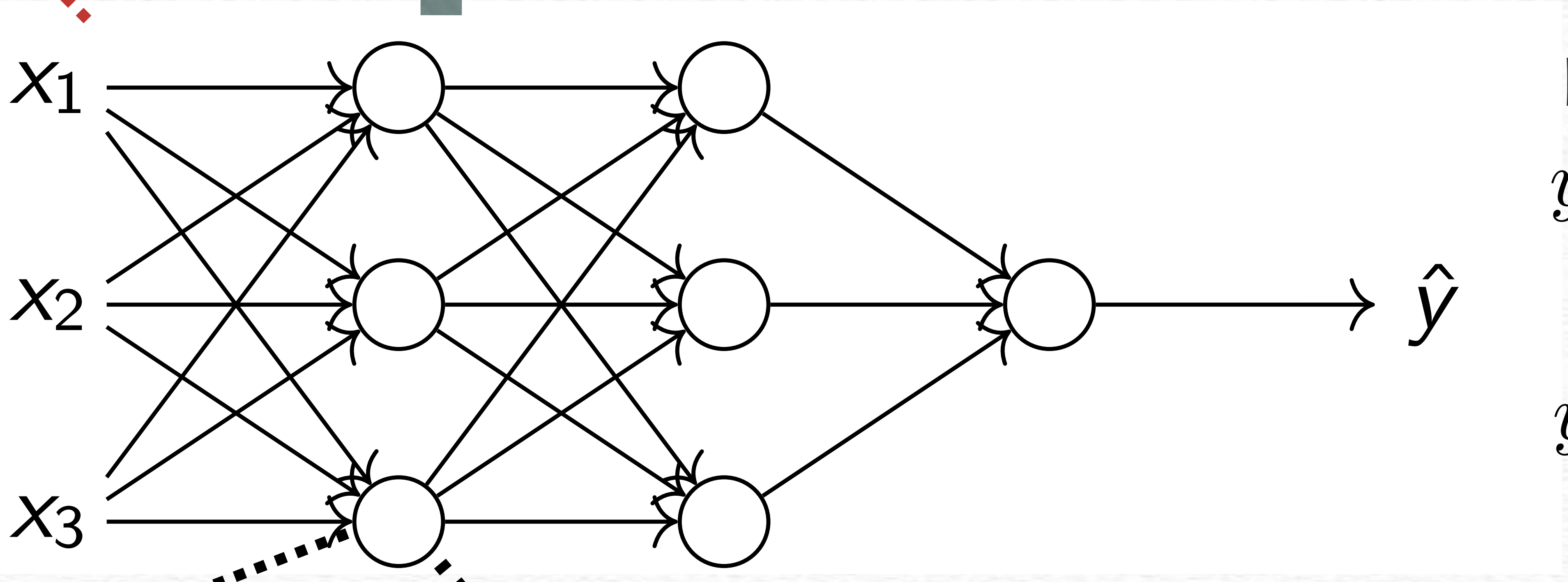
QCD (j+Z(→νν))



output: $\mathbf{w_{ij}}, \mathbf{b_i}$

optimization of loss function

$L(y, \hat{y})$



Higgs

$y = (1, 0)$

QCD

$y = (0, 1)$

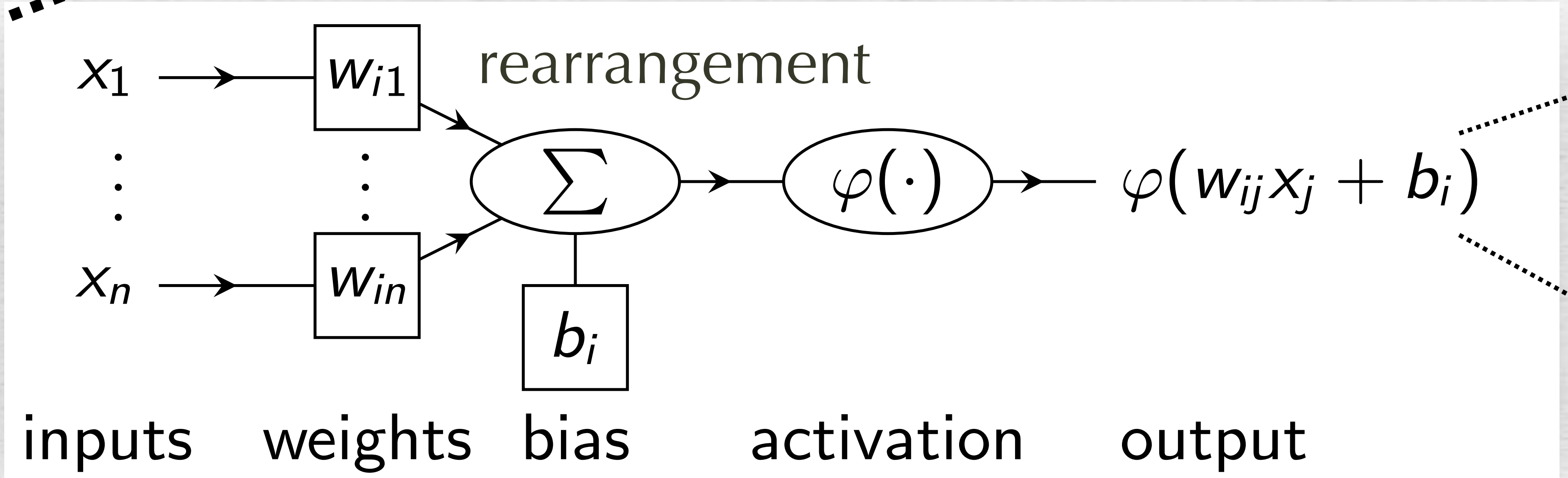
✅expressive power of DL

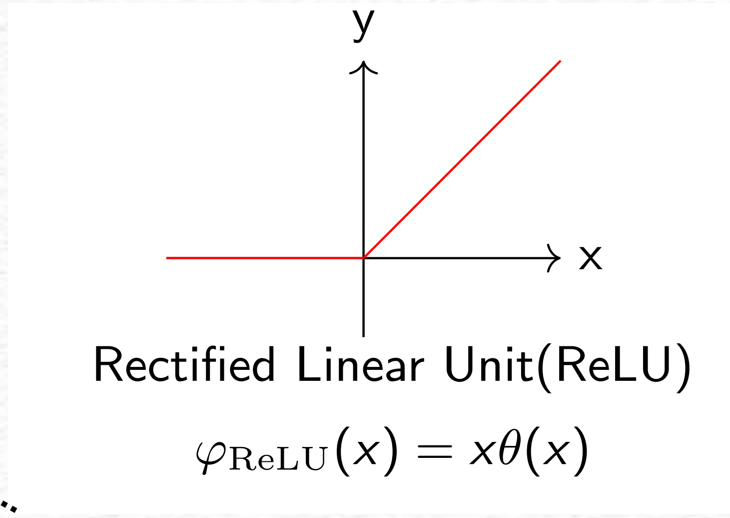
✅learn from data

✅Simple linear algebra + activation

activation function

ϕ: source of non linearity

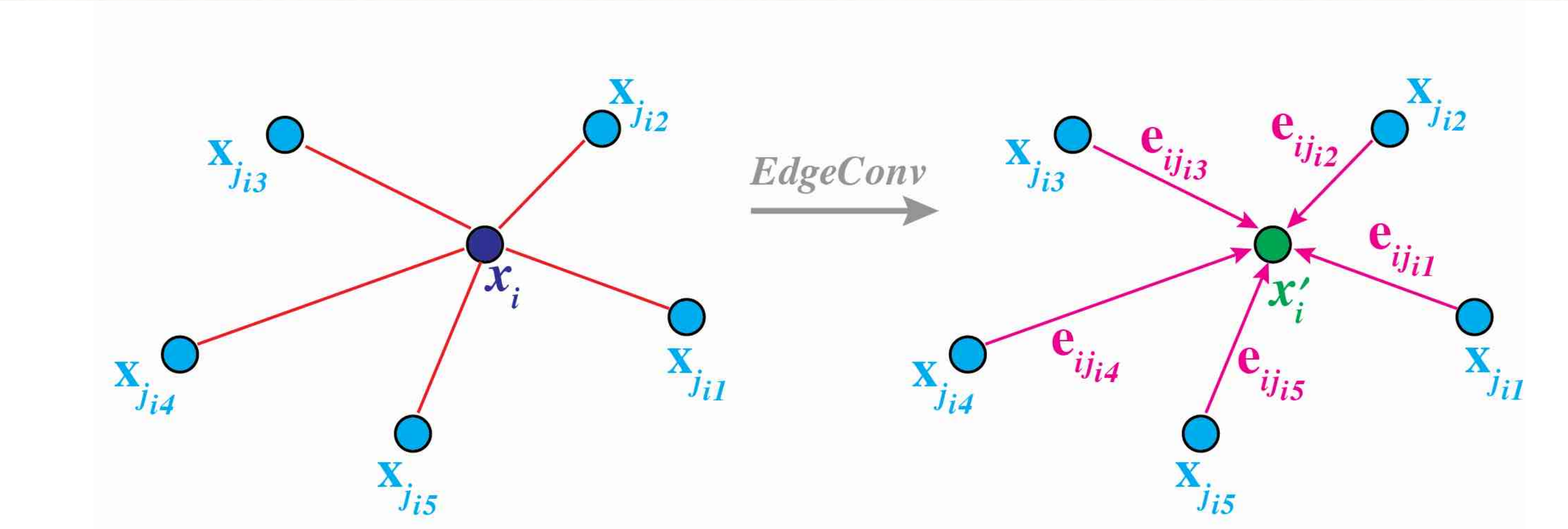




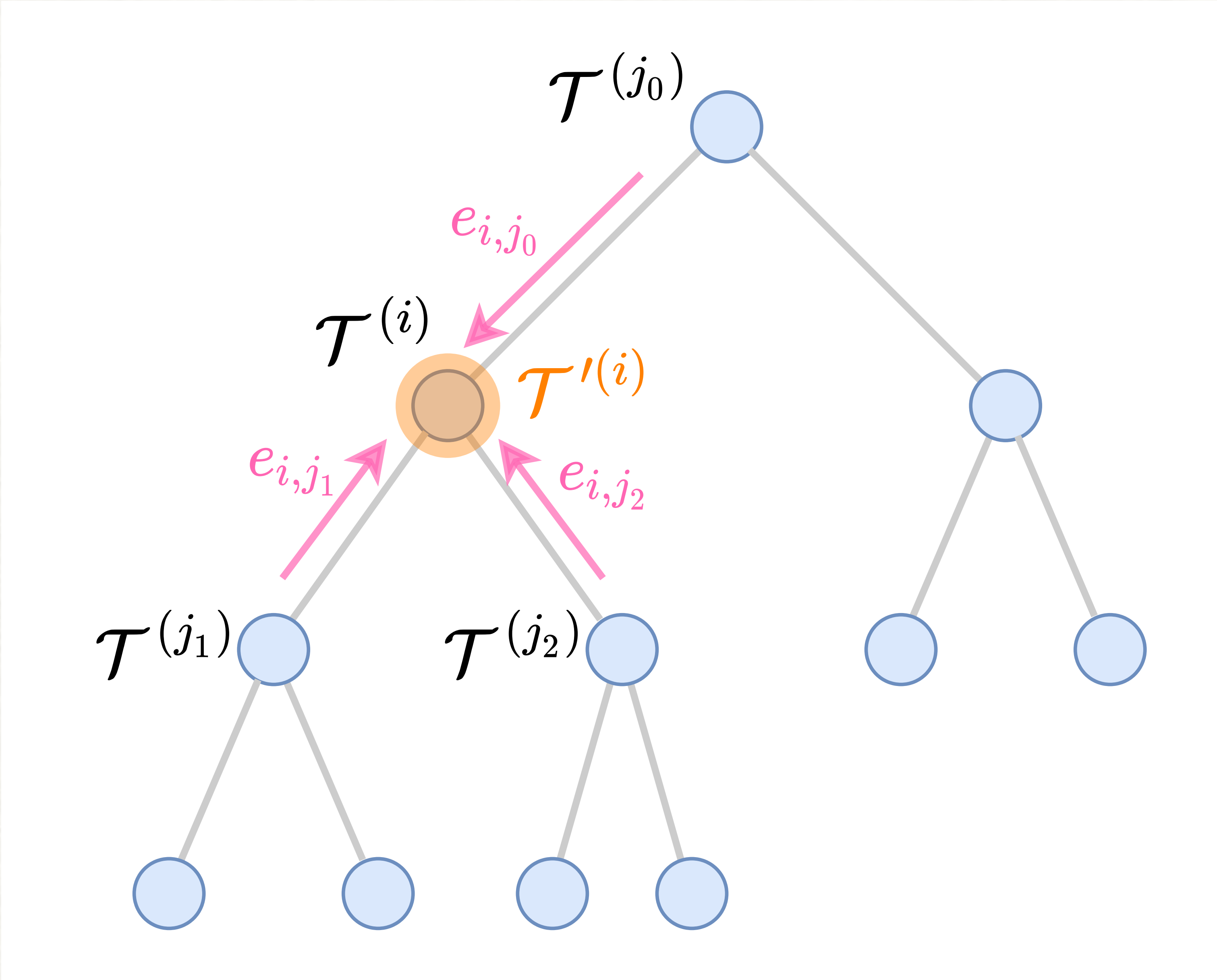
PARTICLE NET(1902.08570) → LUND NET(2012.08526)

Particle NET : Large Nearest neighber→ very large demand on GPU memory
Lund net: Replace Particle information to the jet cluster sequence ~ only 3 nearby particles.

MODEL INDEPENDENT

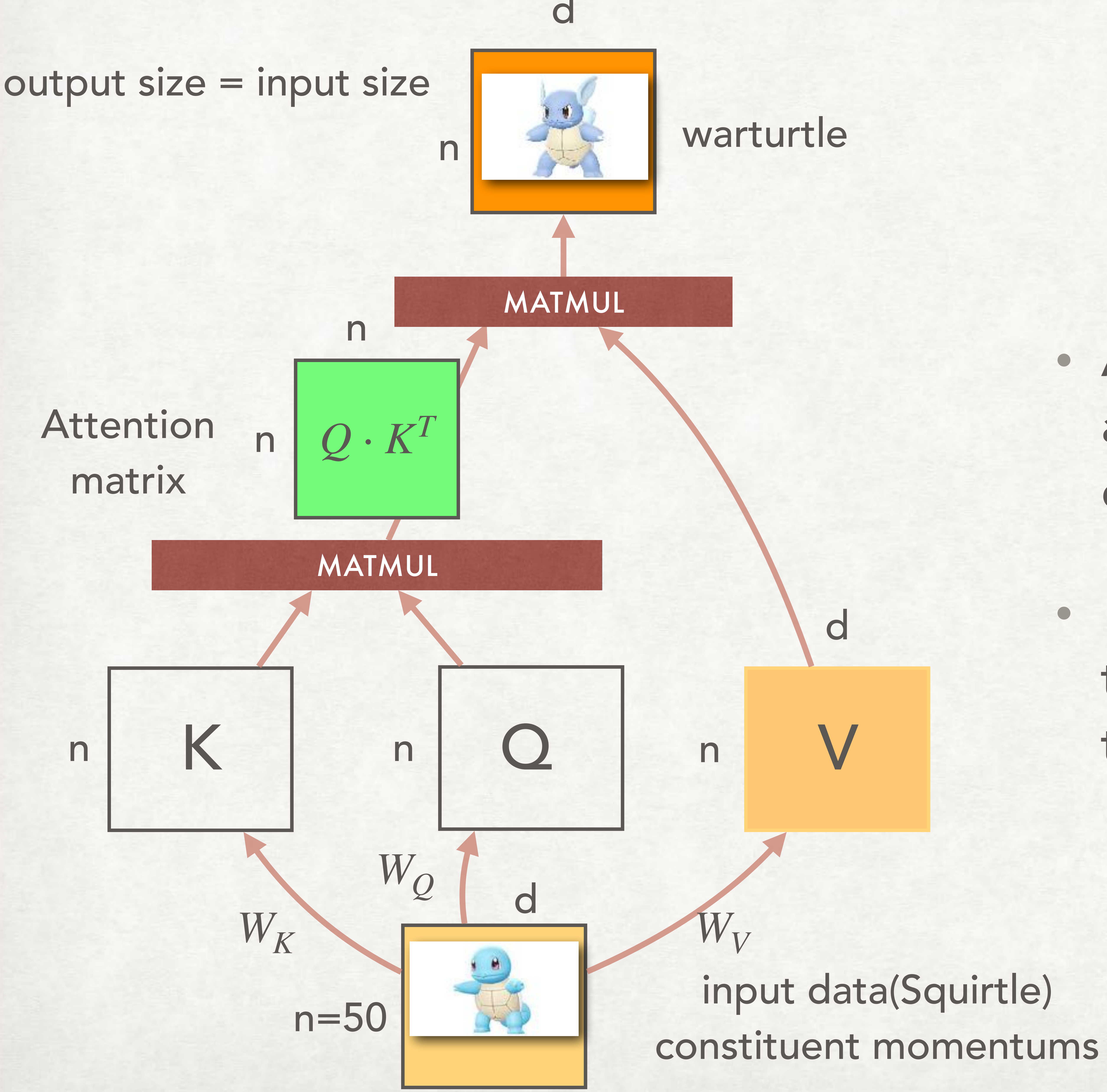


PHYSICS INSIGHT



(a)

"TRANSFORMER" :SELF ATTENTION LAYERS



$$\mathrm{Attention}(Q,K,V) = \mathrm{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

- Attention Matrix mix all features. Higher attention elements indicates important correlations
- transformation V → V' does not change the dimension. Structure of V retained for the next transformation.

CMS will have jet trigger using transformer soon

CONNECTING JET STRUCTURE INFORMATION TO EVENT KINEMATICS

- Non SM Higgs boson (Two Higgs doublet model)
  - pp → H (Heavy Higgs boson) → hh → 4 bjet
  - mH=600-2000 GeV, mh=125.11GeV
  - Delphes background pp → 4b and pp →tt
  - two fatjets (radius R=1.0) pT cut on the fatjet P_{T1}>450GeV P_{T2}> 250GeV.

    ATLAS *Phys. Rev. D*, 105(9):092002, 2022.
  - double b tags for each fatjet (Delphes 80% tagging efficiency) 250GeV >M(J)>50GeV
  - **no pileup (theorist job)**

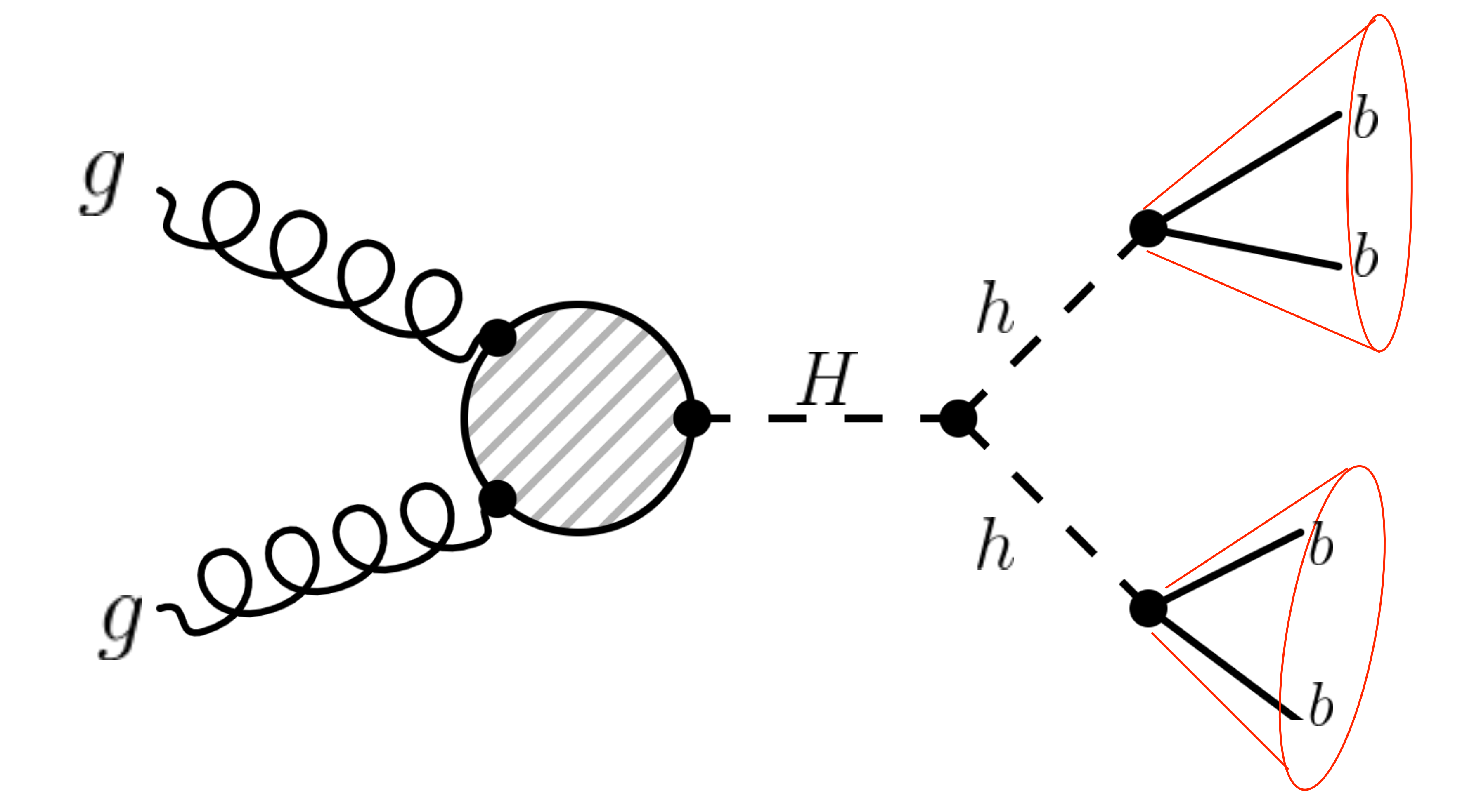
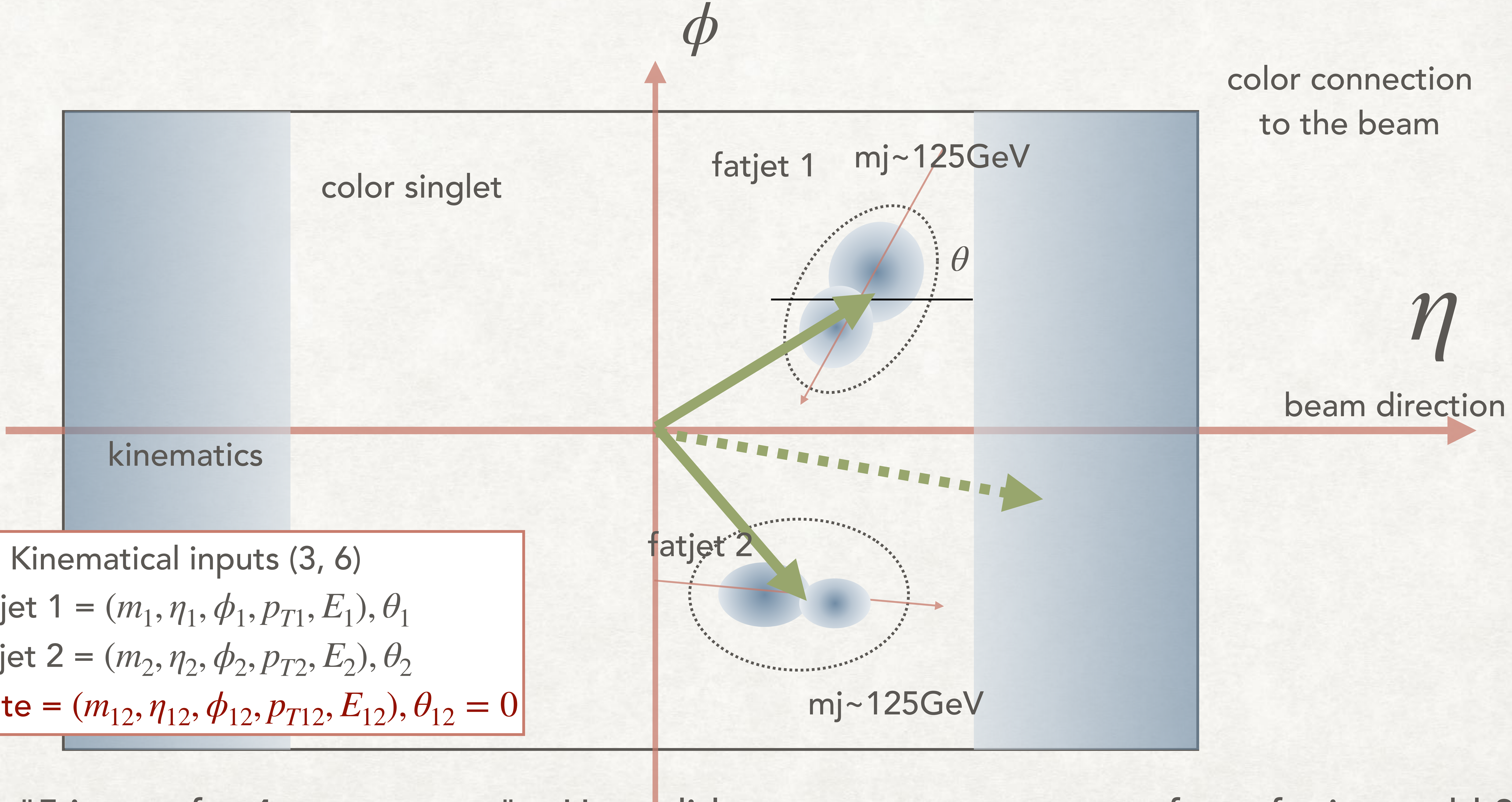


Figure 2: Feynman diagram for the signal process.

$$
\begin{aligned}
V_\phi = {} & m_{11}^2(\phi_1^\dagger\phi_1) + m_{22}^2(\phi_2^\dagger\phi_2) - \left[m_{12}^2(\phi_1^\dagger\phi_2) + \mathrm{h.c.}\right] \\
& + \lambda_1(\phi_1^\dagger\phi_1)^2 + \lambda_2(\phi_2^\dagger\phi_2)^2 + \lambda_3(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_4(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) \\
& + \frac{1}{2}\left[\lambda_5(\phi_1^\dagger\phi_2)^2 + \left[\lambda_6(\phi_1^\dagger\phi_1) + \lambda_7(\phi_2^\dagger\phi_2)\right](\phi_1^\dagger\phi_2) + \mathrm{H.c.}\right] .
\end{aligned}
$$

INPUT TO NETWORK : EVENT KINEMATICS



Kinematical inputs (3, 6)

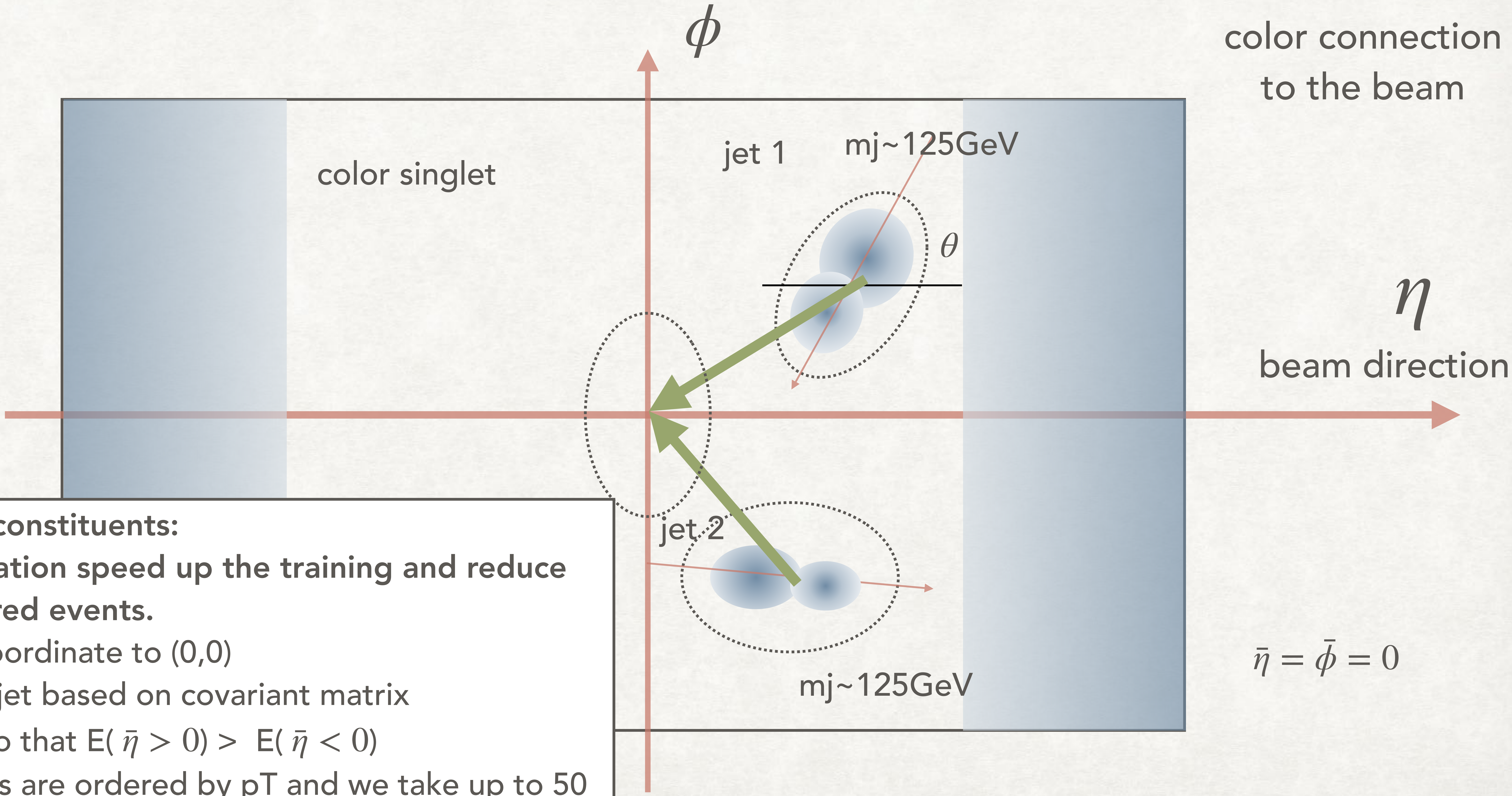
fatjet 1 = $(m_1, \eta_1, \phi_1, p_{T1}, E_1), \theta_1$

fatjet 2 = $(m_2, \eta_2, \phi_2, p_{T2}, E_2), \theta_2$

H candidate = $(m_{12}, \eta_{12}, \phi_{12}, p_{T12}, E_{12}), \theta_{12} = 0$

NOTE : "5 inputs for 4 momentum" , H candidate momentum as sum of two fat jets, add **θ**,

INPUT TO NETWORK: JET SUBSTRUCTURE INFO



up to 50 constituents:
Regularization speed up the training and reduce the required events.

1. shift coordinate to (0,0)
2. rotate jet based on covariant matrix
3. flip η so that E($\bar{\eta} > 0$) > E($\bar{\eta} < 0$)

4. particles are ordered by pT and we take up to 50

$p_i = (\bar{\eta}_i, \bar{\phi}_i, p_{Ti}, \log p_{Ti})$ → (50, 4) data

HOW TO COMBINE JET STRUCTURE AND EVENT KINEMATICS

Naive approach "simple concatenation"

2311.16674[hep-ph] K. Ban, KC Kong, M Park,S.C. Park

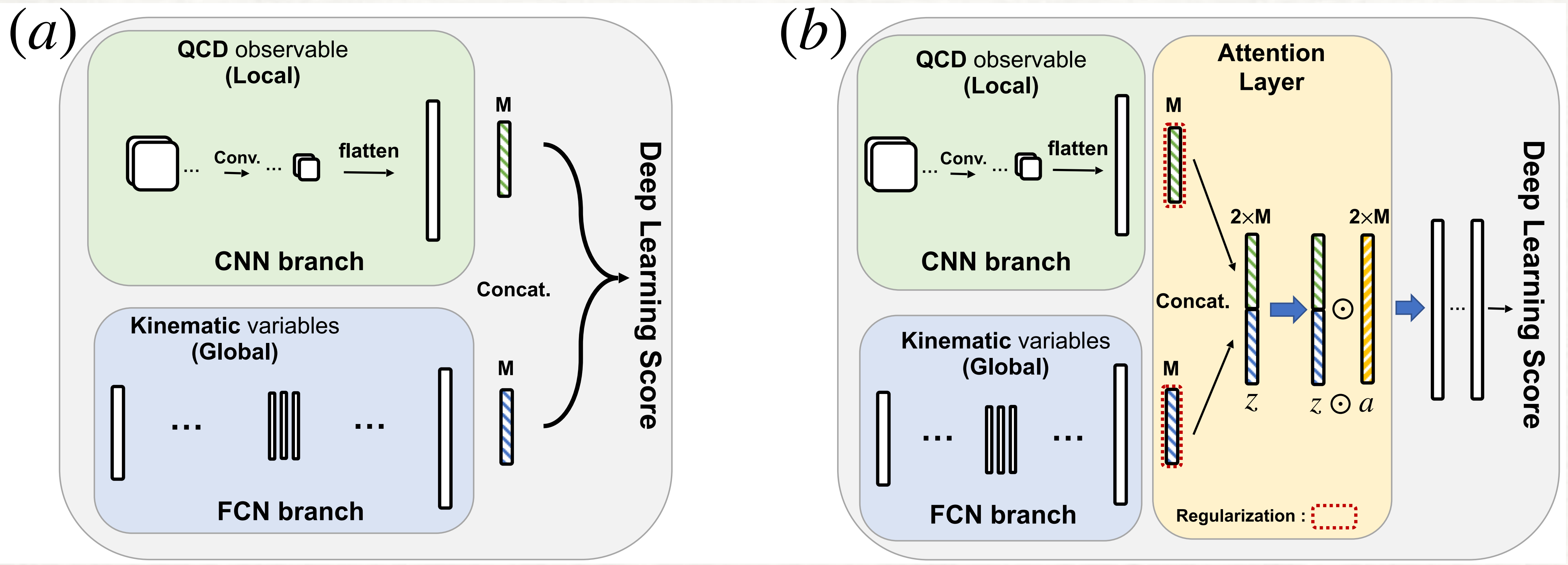
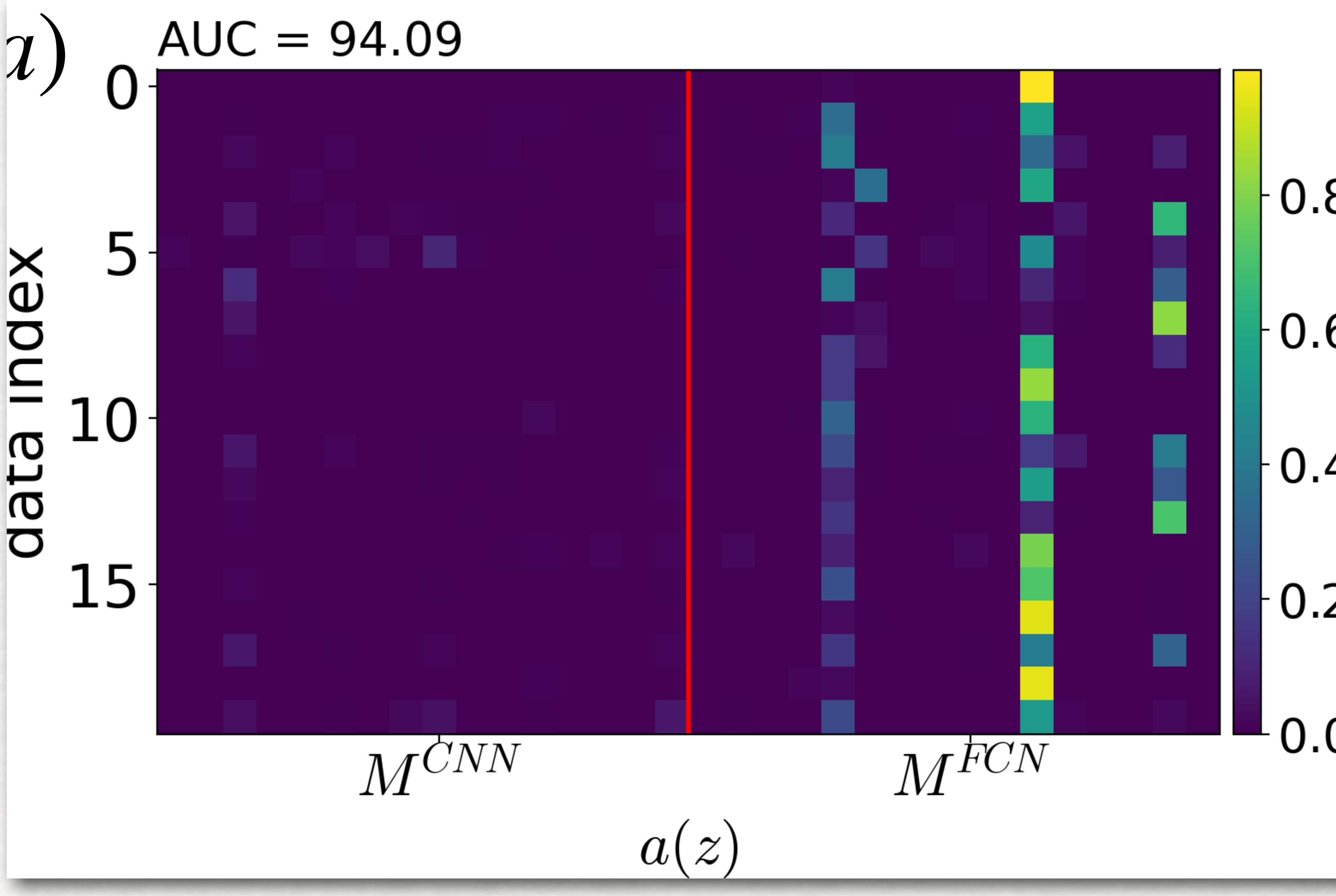


FIG. 2. The schematic plots for neural network structures: (a) conventionally used one in previous studies only with concatenation and (b) our proposed one with a regularized attention mechanism.



a) [Jet momentum (parton momentum)]+[jet concatenation] does not work.

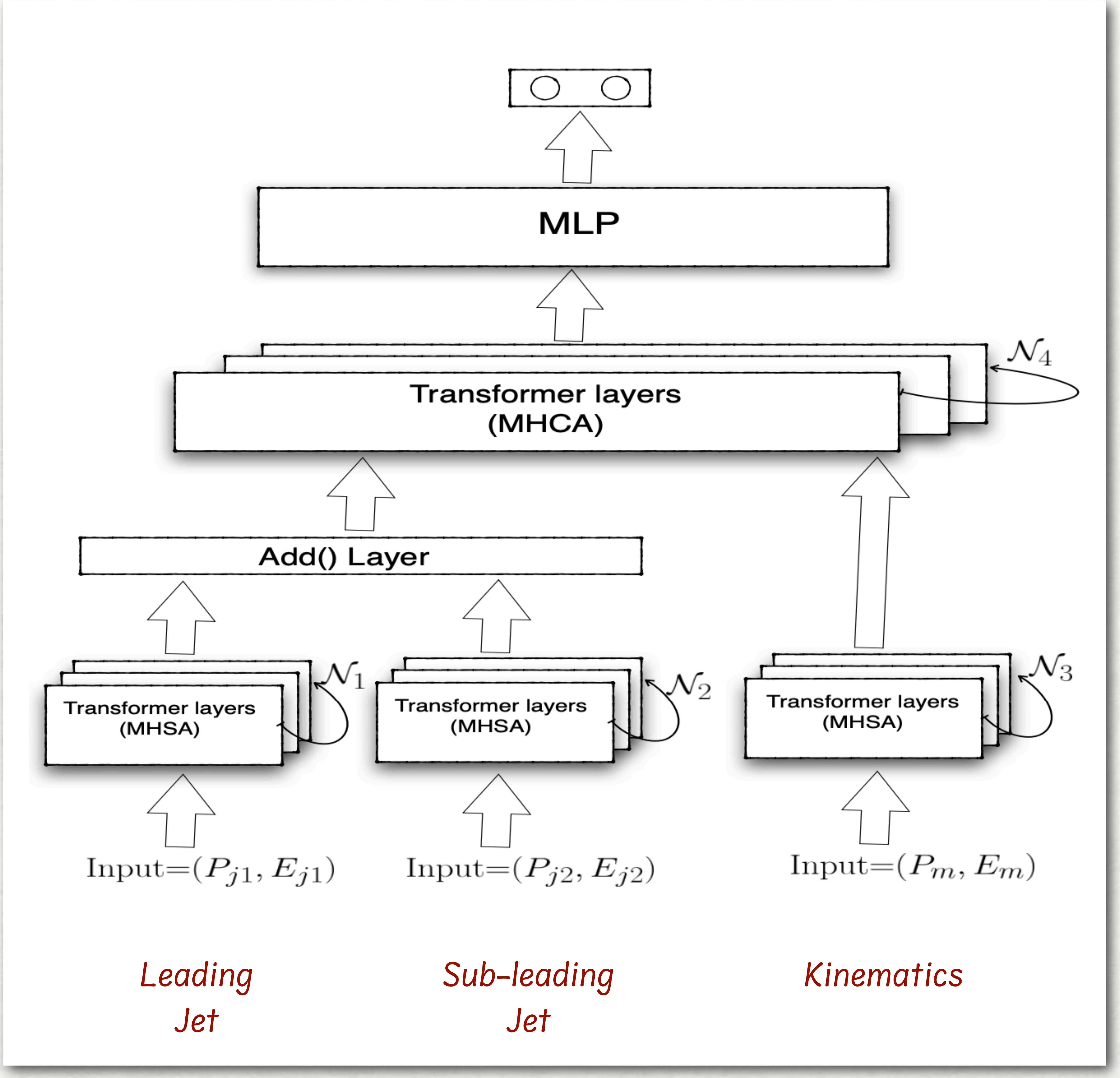
because of imbalance of "importance" of two information → the minor one can be ignored in the training.

Pre-training and freeze substructure analysis? We would loose the correlation to global kinematics.

OUR CROSS ATTENSION MODEL

multihead
cross attention layers

multihead
self attention layers



step 2 :Cross attention

transform jet kin by
cross Att. [substracture]x [jet kin]

step 1 : Self attention

[substructure]x[substructure]

[jet kin] x [jet kin]

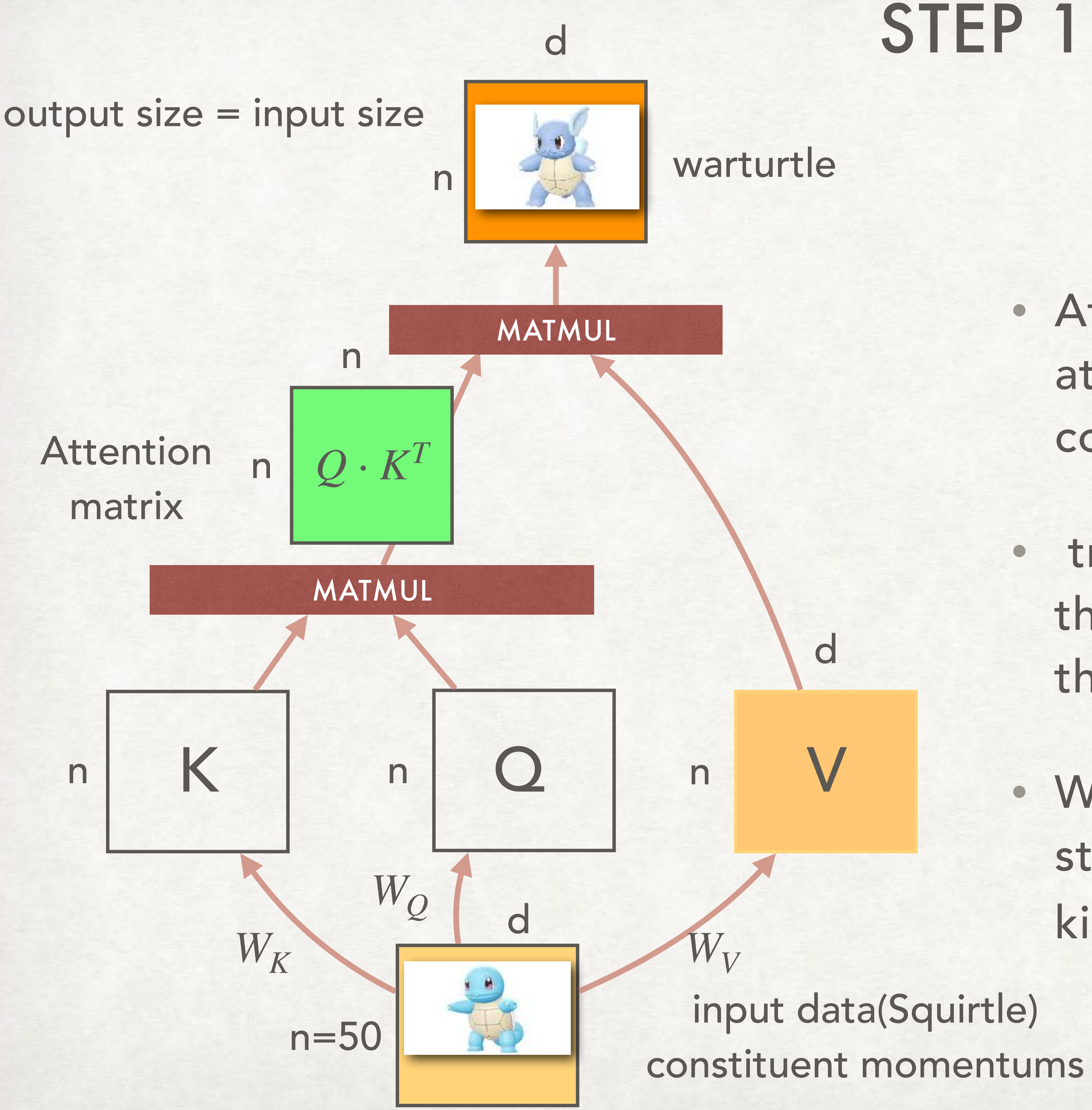
TAKEAWAYS

- use **"cross attention"** when you combine the "high scale information" to the "low energy scale", because cross attention layer gives extra emphasis to the information linked to the high energy kinematics.

- **skip connection and Interpretation :** Skip connection helps to maintain some connection to the inputs

- More Physics: Heavy particles decay into colored particles (discovery, spin, color structure?) Cross attention network probably more useful to resolve correlation of jet structures.

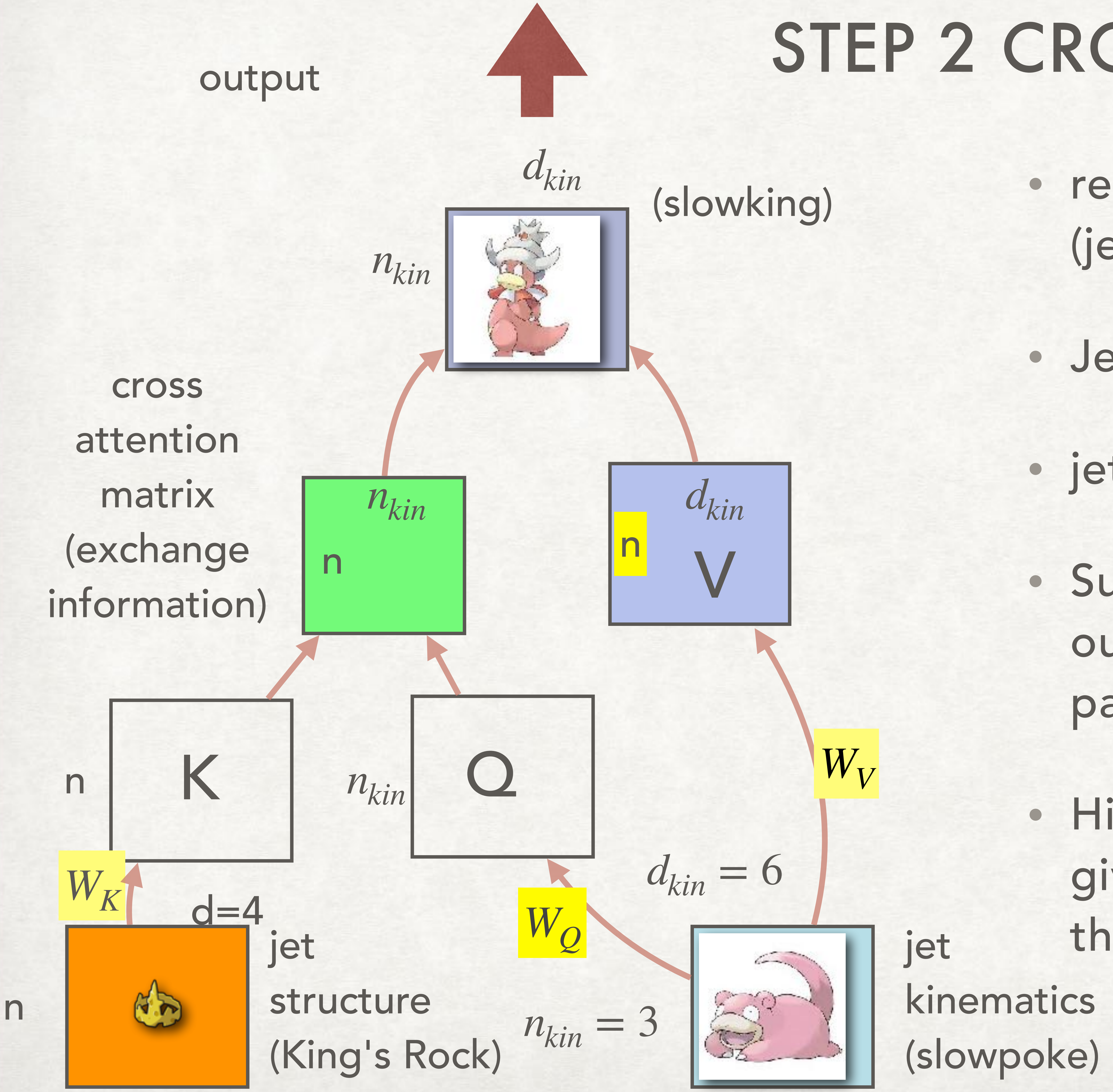
STEP 1 SELF ATTENTION LAYERS



$$\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$

- Attention Matrix mix all features. Higher attention elements indicates important correlations
- transformation V → V' does not change the dimension. Structure of V retained for the next transformation.
- We adopt 50x50 self attention for jet structurre and 3x3 self attention for jet kinematics, with $n_{head} = 5$

STEP 2 CROSS ATTENTION LAYERS

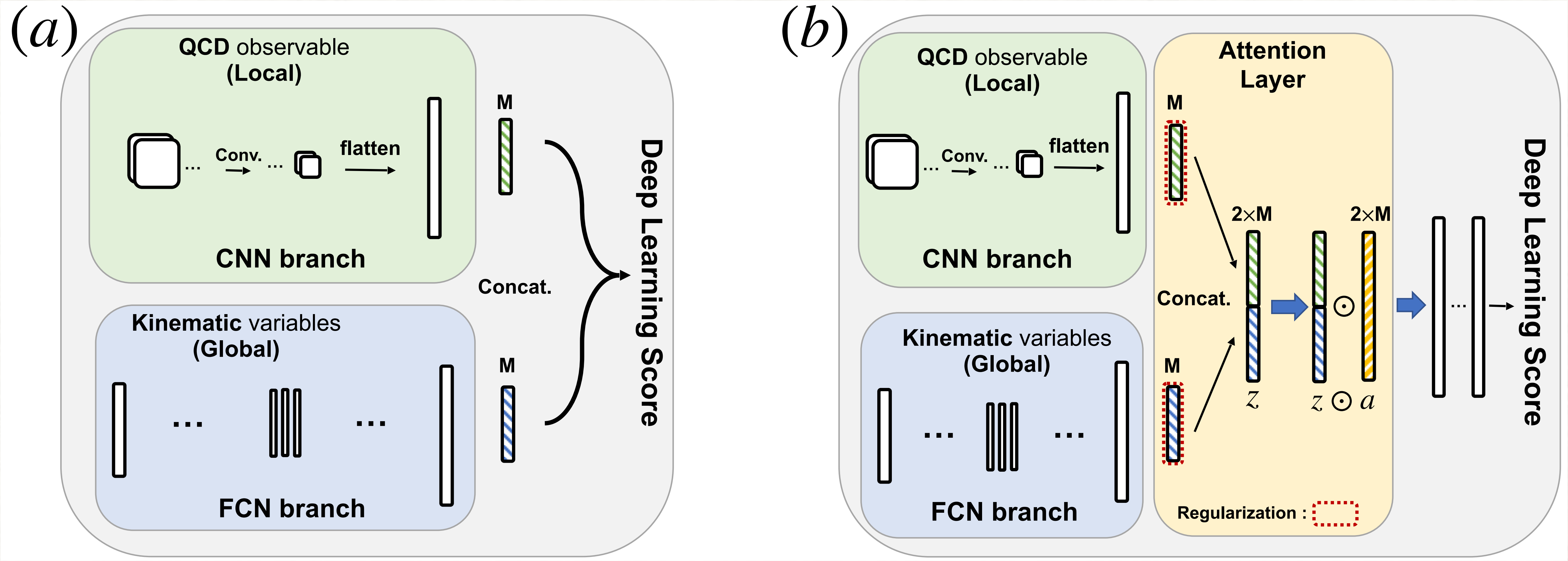


- restrict network to cross attention (jet kin) x (jet str.)
- Jet momentum : hard physics of partons Q , V
- jet substructure: parton shower, hadronization K
- Substructure output K and Jet kinematics output Q make cross attention matrix. The pairs update V (jet Kin)
- High scale feature relevant for classification gives extra weight to the corresponding jets though backward propagation

COMPARISON WITH OTHER APPROACH

Naive approach "simple concatenation"

2311.16674[hep-ph] K. Ban, KC Kong, M Park,S.C. Park



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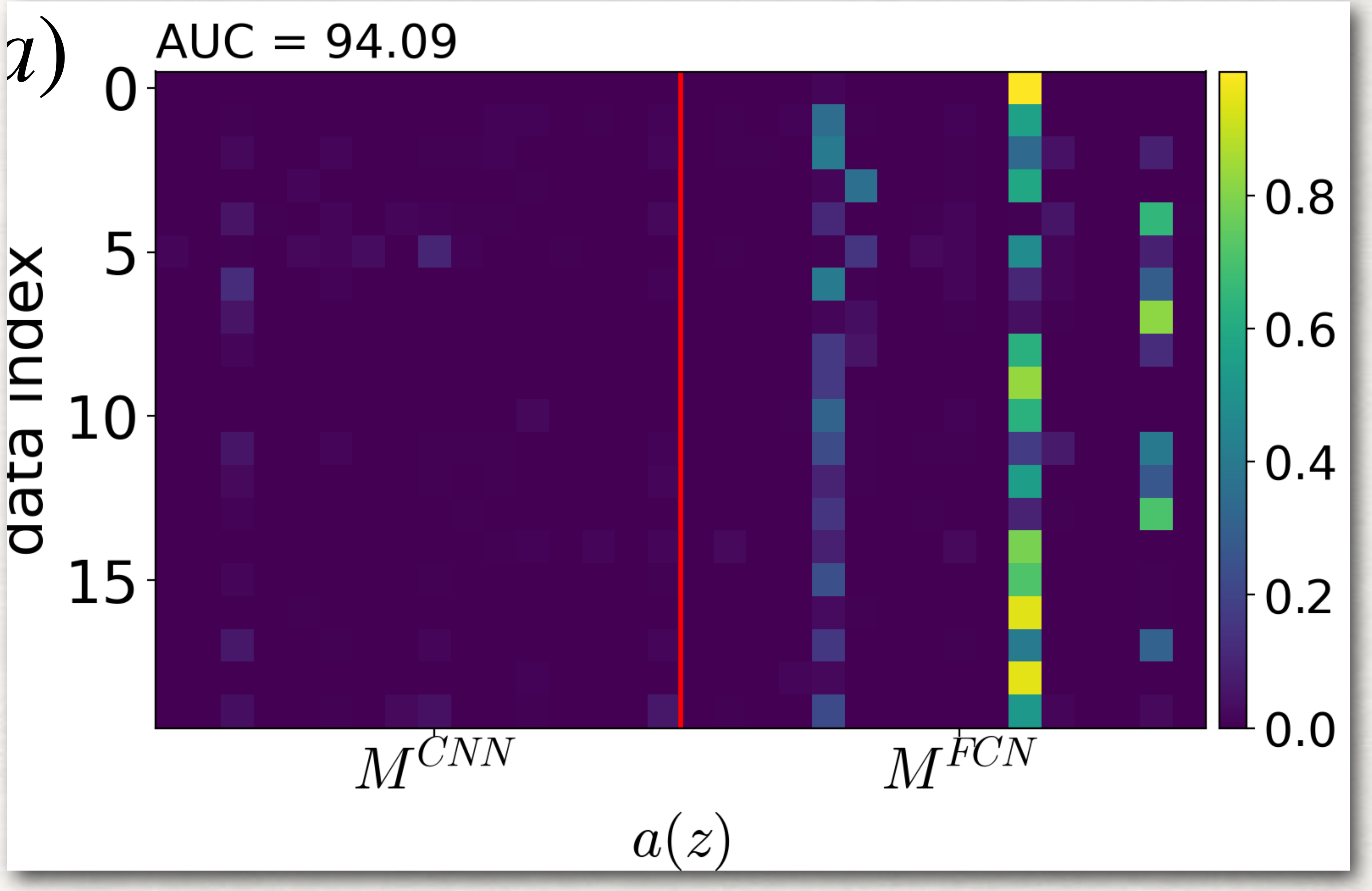


our network kill this term
and keep off-diagonal part only

(b) self attention matrix of combined information

$$A\,V = \begin{pmatrix} Q(Sub) \times K(Sub\,) & Q(Kin \times K(Sub) \\ Q(Sub) \times K(Kin) & Q(Kin)\,K(Kin) \end{pmatrix} V = \boxed{Q(kin)\,K(kin)\,V(kin)} + \dots.$$

PHYSICS BEHIND THE NETWORK

Classification is "probablity ratio estimation"

- a jet:

P(hadrons in jets | parton or jet) = $P(\{x_i\} \,|\, y)$

- a fatjet or a jet with substructure

$$P(\{x_i\} \,|\, \{y_\alpha\})$$

- cross attention: two fatjets in an event (factorization)

$$P(\{x_i\}, \{x_j'\}, \{y_\alpha\}, \{y_\beta'\}) \sim P(\{x_i\} \,|\, \{y_\alpha\}) P(\{x_i'\} \,|\, \{y_\beta'\})\ P(\{y_\alpha\ , y_\beta'\})$$

- our model also allows

$$P(\{x_i\}, \{x_j'\}, \{y_\alpha, y_\beta'\}) \sim P(\{x_i\} \,|\, \{y_\alpha, y_\beta'\}) P(\{x_i'\} \,|\, \{y_\alpha, y_\beta'\})\ P(\{y_\alpha, y_\beta'\})$$

IMPROVEMENT USING CROSS ATTENTION

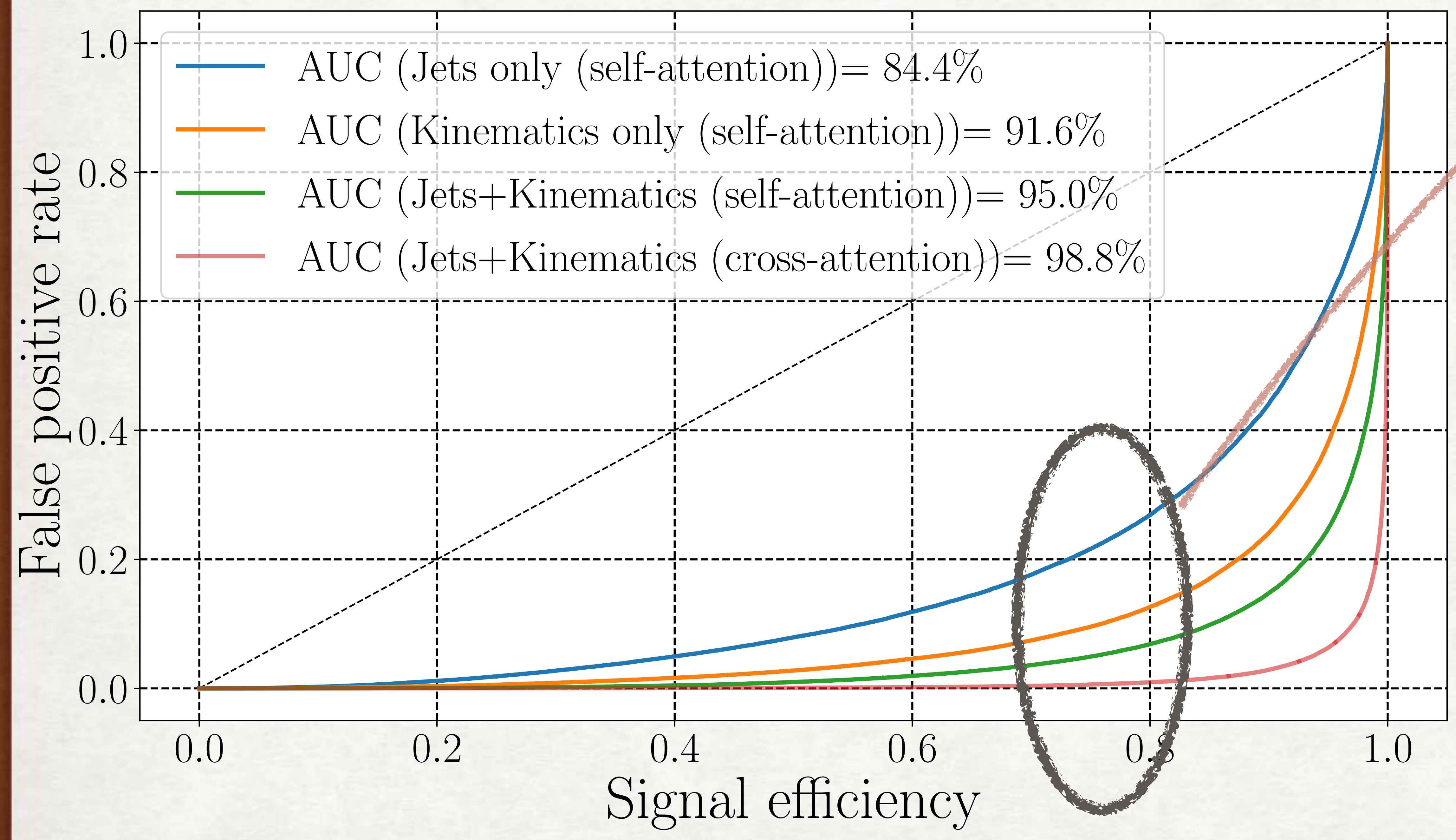
green: self attention of Jet str. and Kin

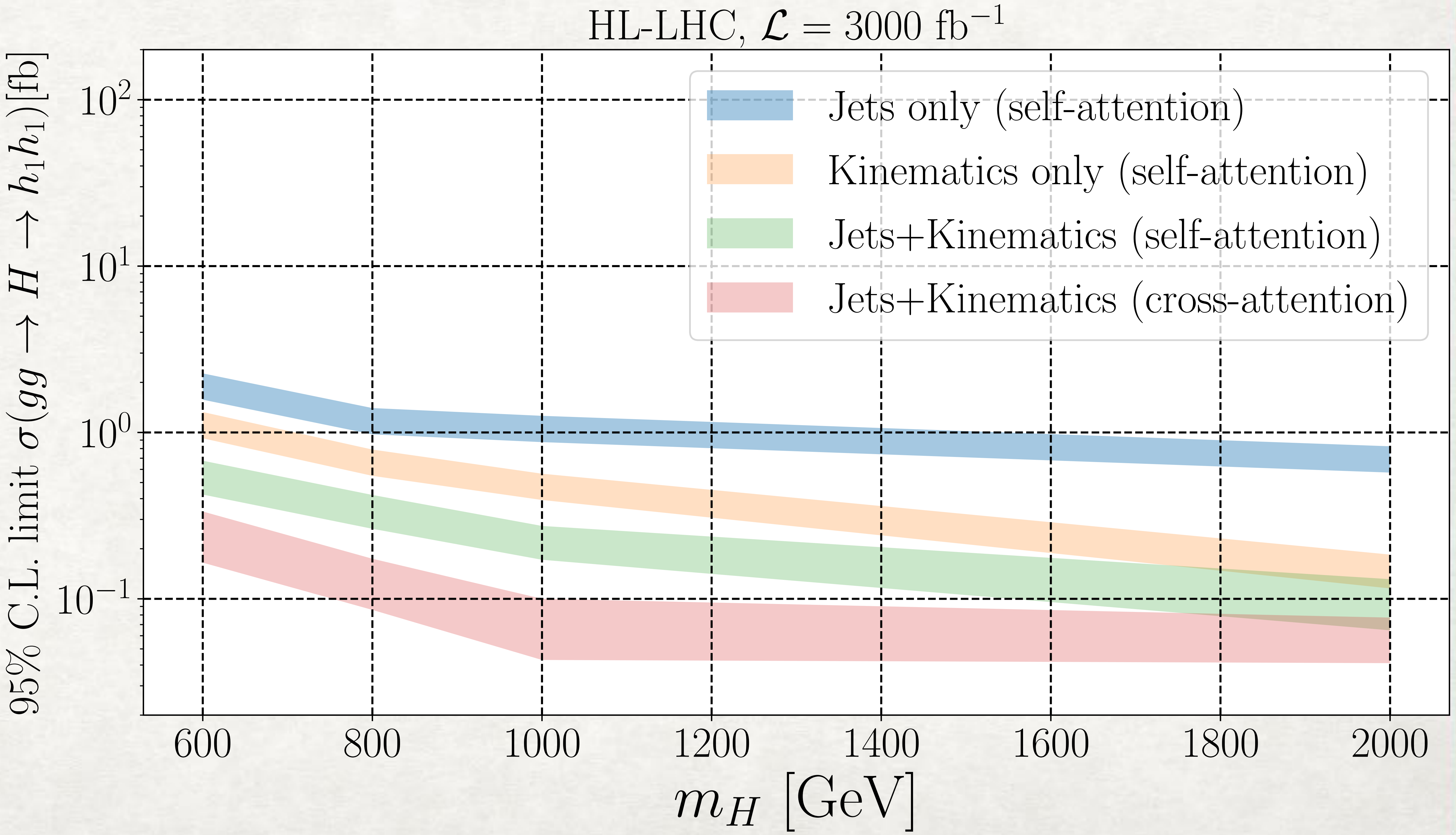
→ concatenate and MLP

red line : cross attention

factor 5 improvement at the same acceptance.

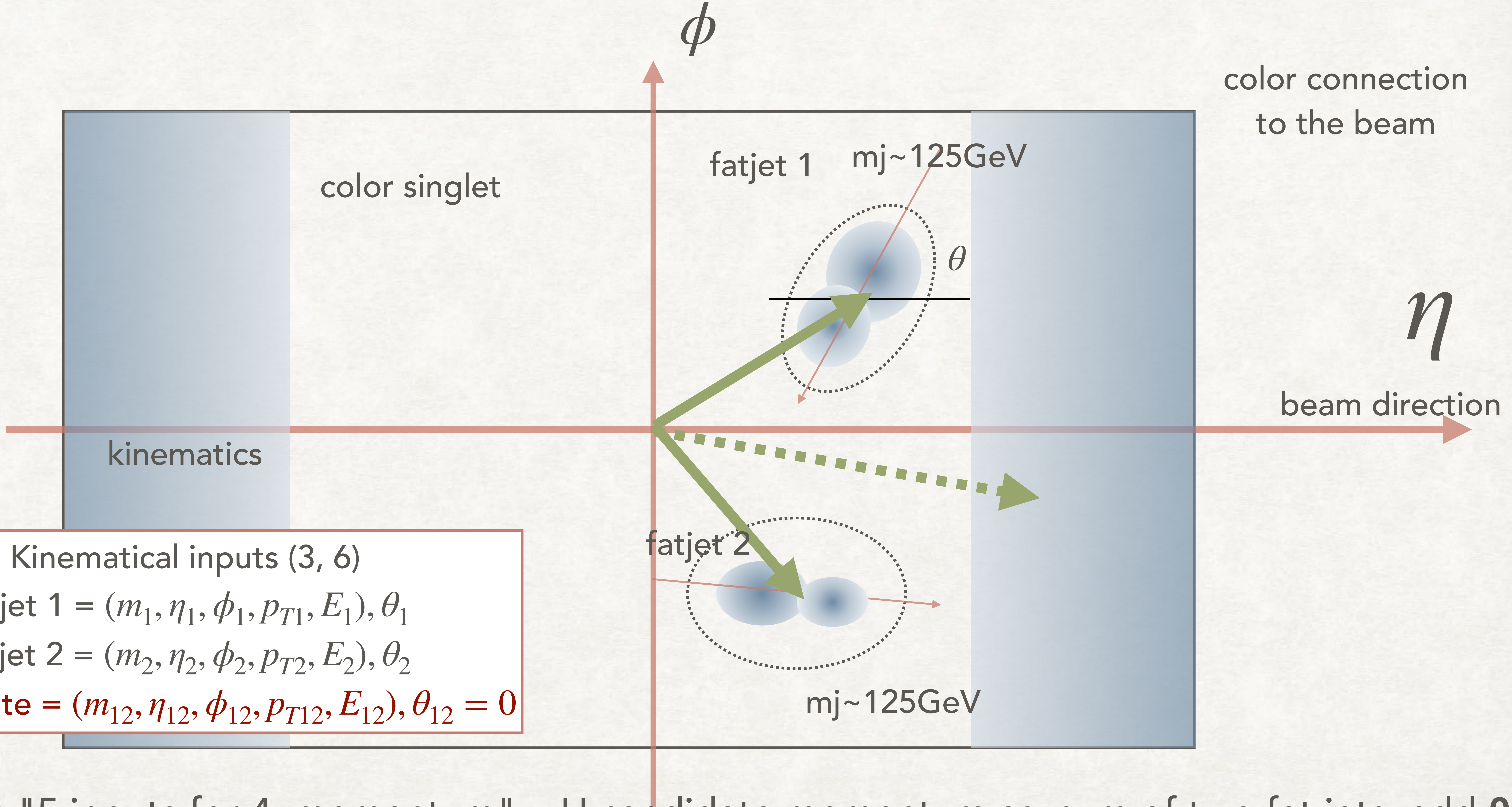
Simple estimation of the upper limits





Cross attention improve the rejection efficiency significantly

INPUT TO NETWORK : EVENT KINEMATICS



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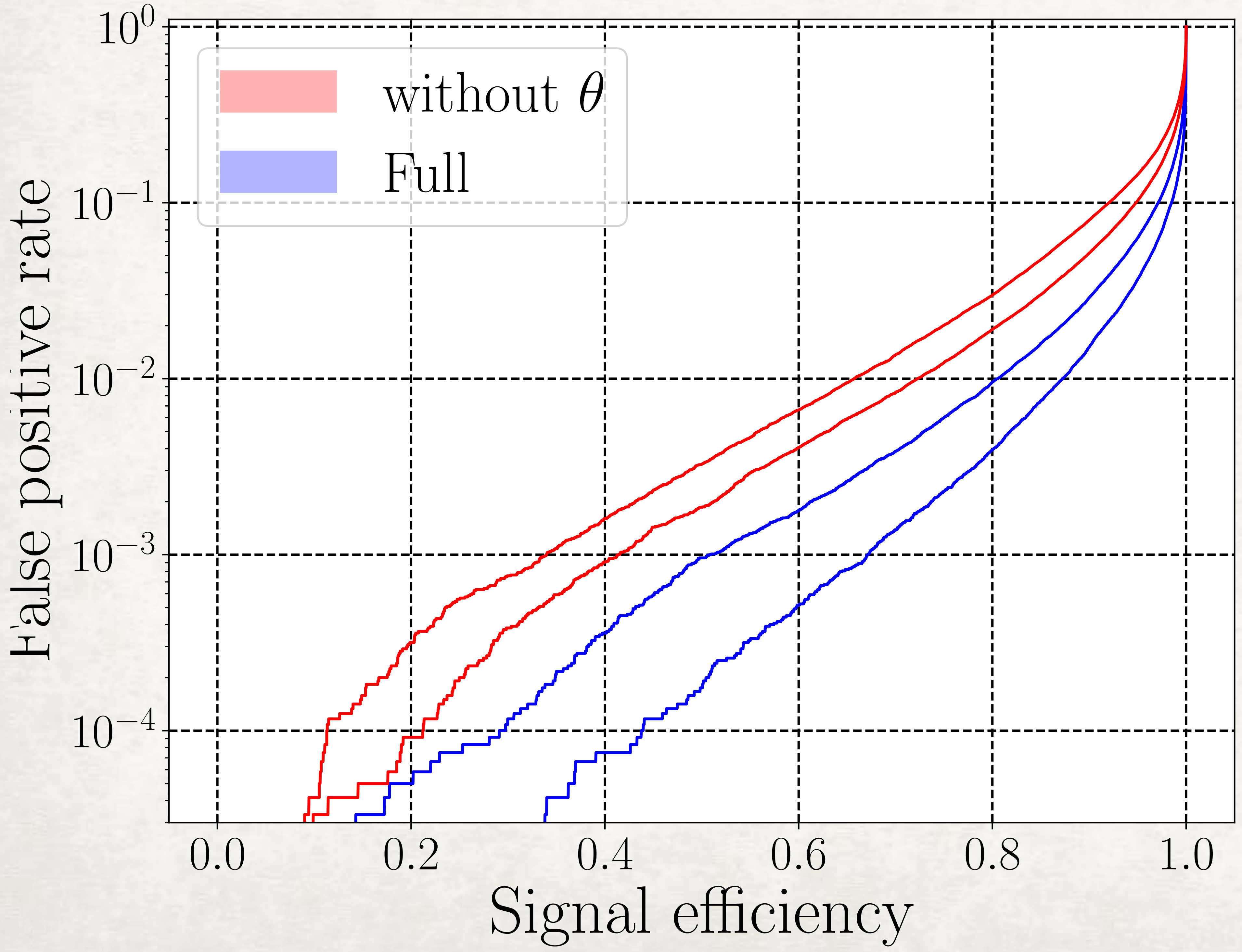
NOTE : "5 inputs for 4 momentum" , H candidate momentum as sum of two fat jets, add **θ**,

ROLE OF θ

minor

large improvement

	Kinematics	Kin +θ	jet str.+kin	jet str +Kin + θ
ROC	91.01%	91.6	97.23-98.16	98.68-99.28

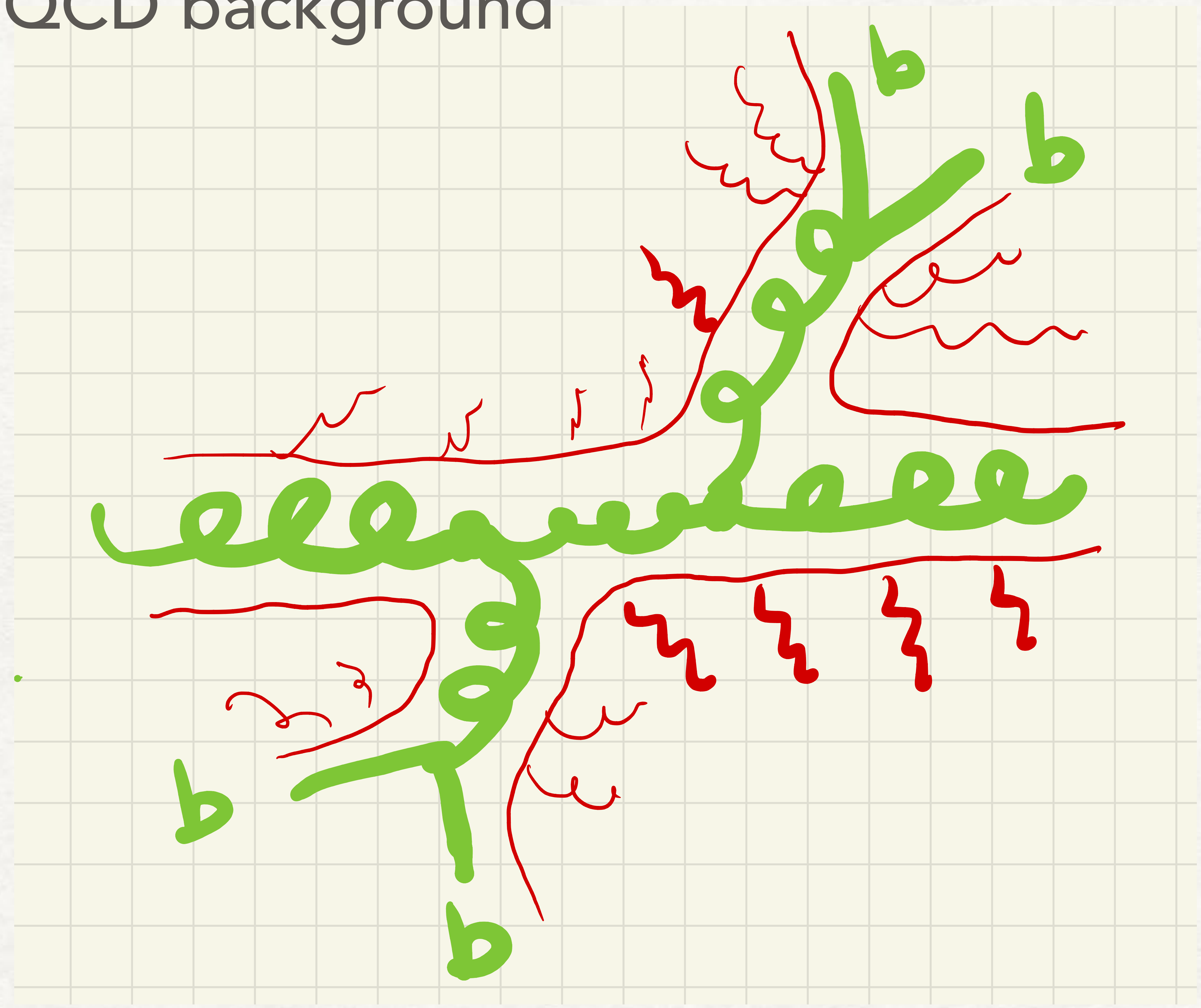


adding rotation angle θ improves classification when both jet str. and kinematical information available.

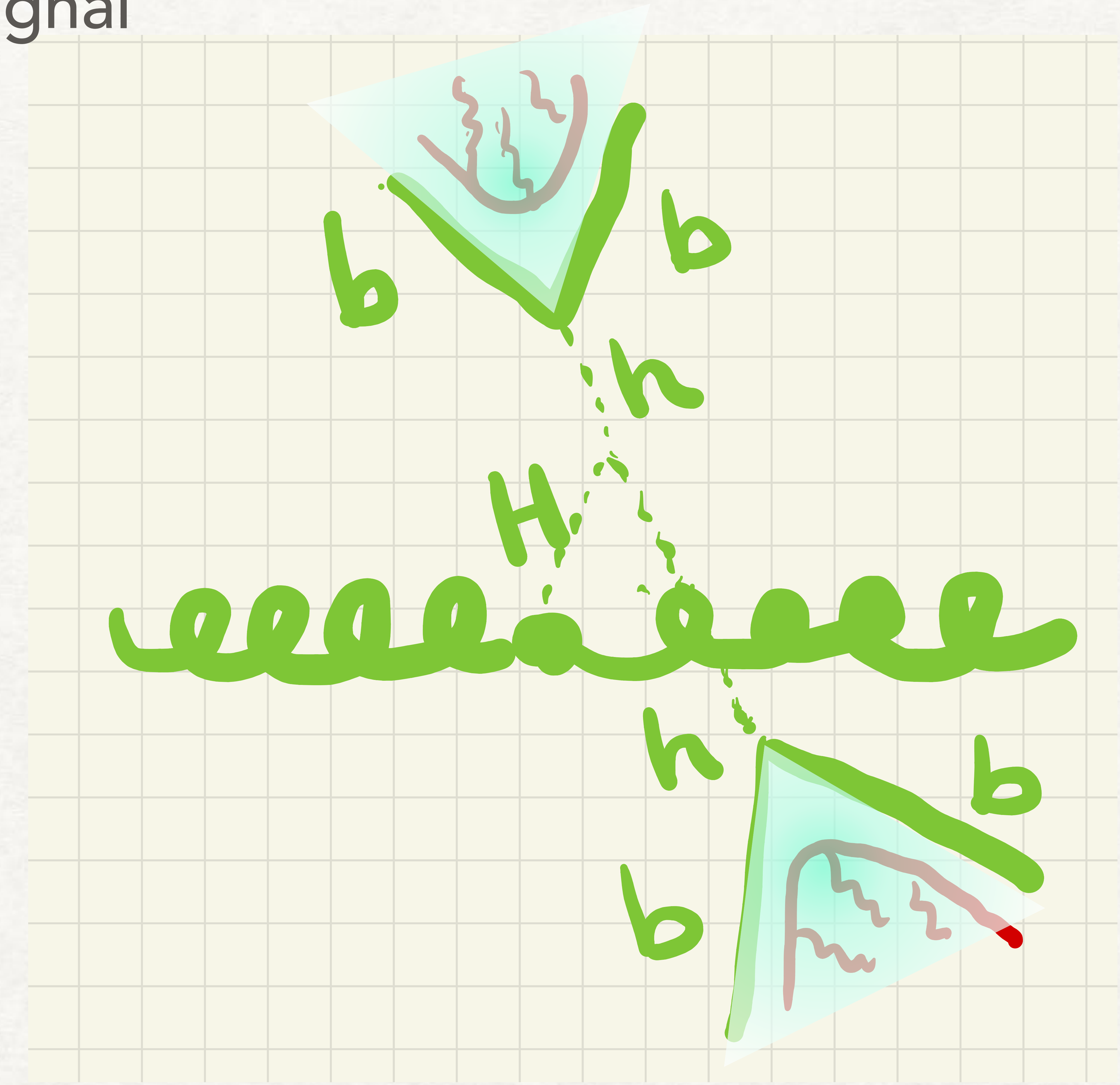
We are working to identify the origin.
(color connection? momentum resolution?)

event color structure

QCD background



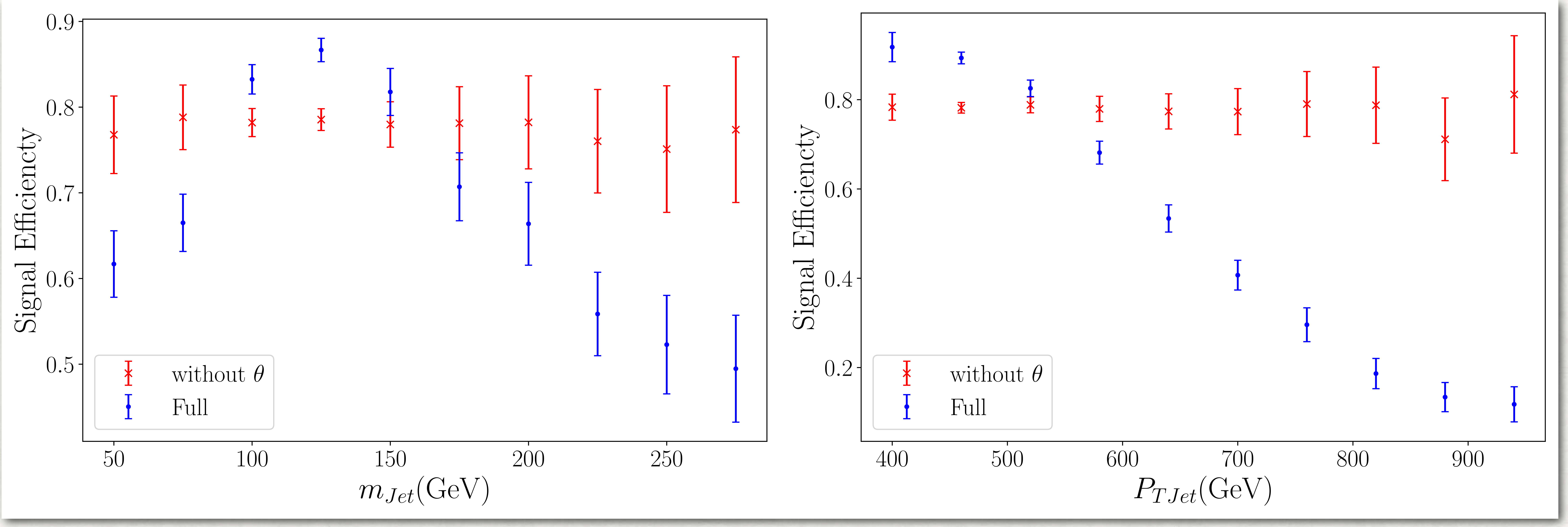
signal



For QCD and top event, fatjets are likely color connected to the other activities of the event

Higgs bosons are color isolated.

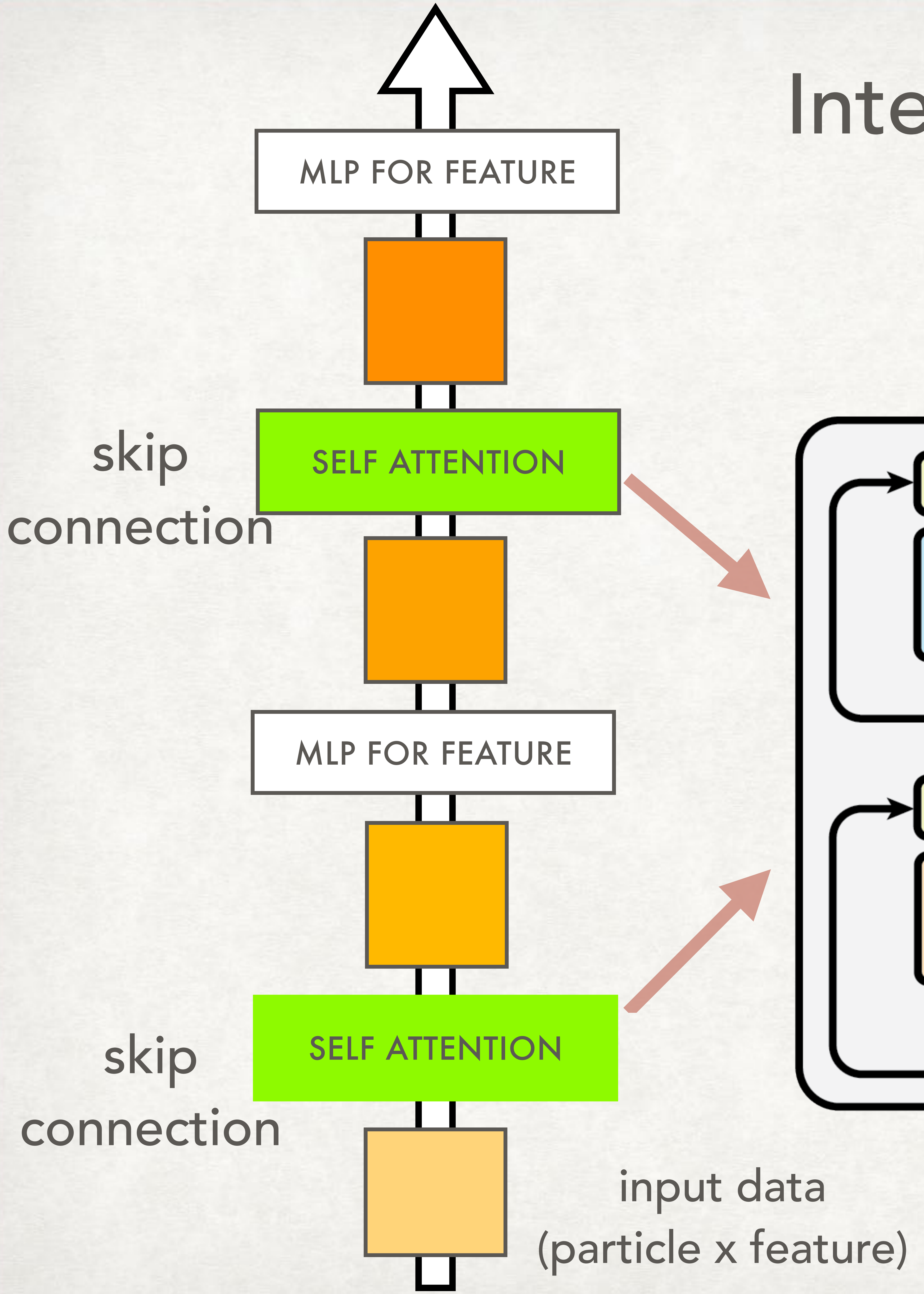
SOME SIGNAL SELECTION EFFICIENCY

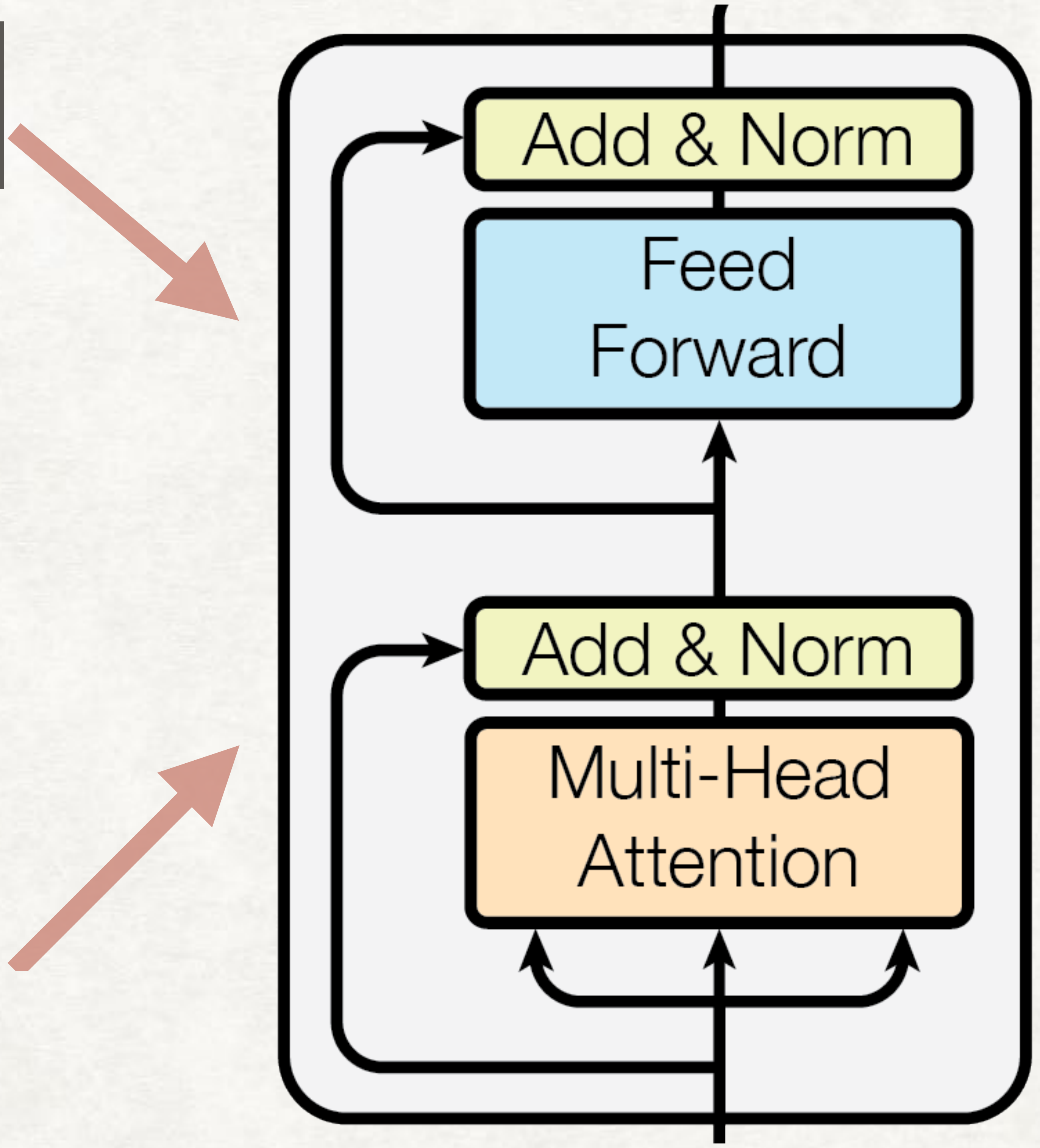


better selection of Higgs mass

rejecting high PT events

Interpretation and Skip Connection





- Deep Learning suffers low interpretability and it is always annoying.
- skip connection of attention blocks $x_i' = x_i + \Phi_i(x)$ helps connecting input data to extracted feature(transformed quantity) in **some level.**

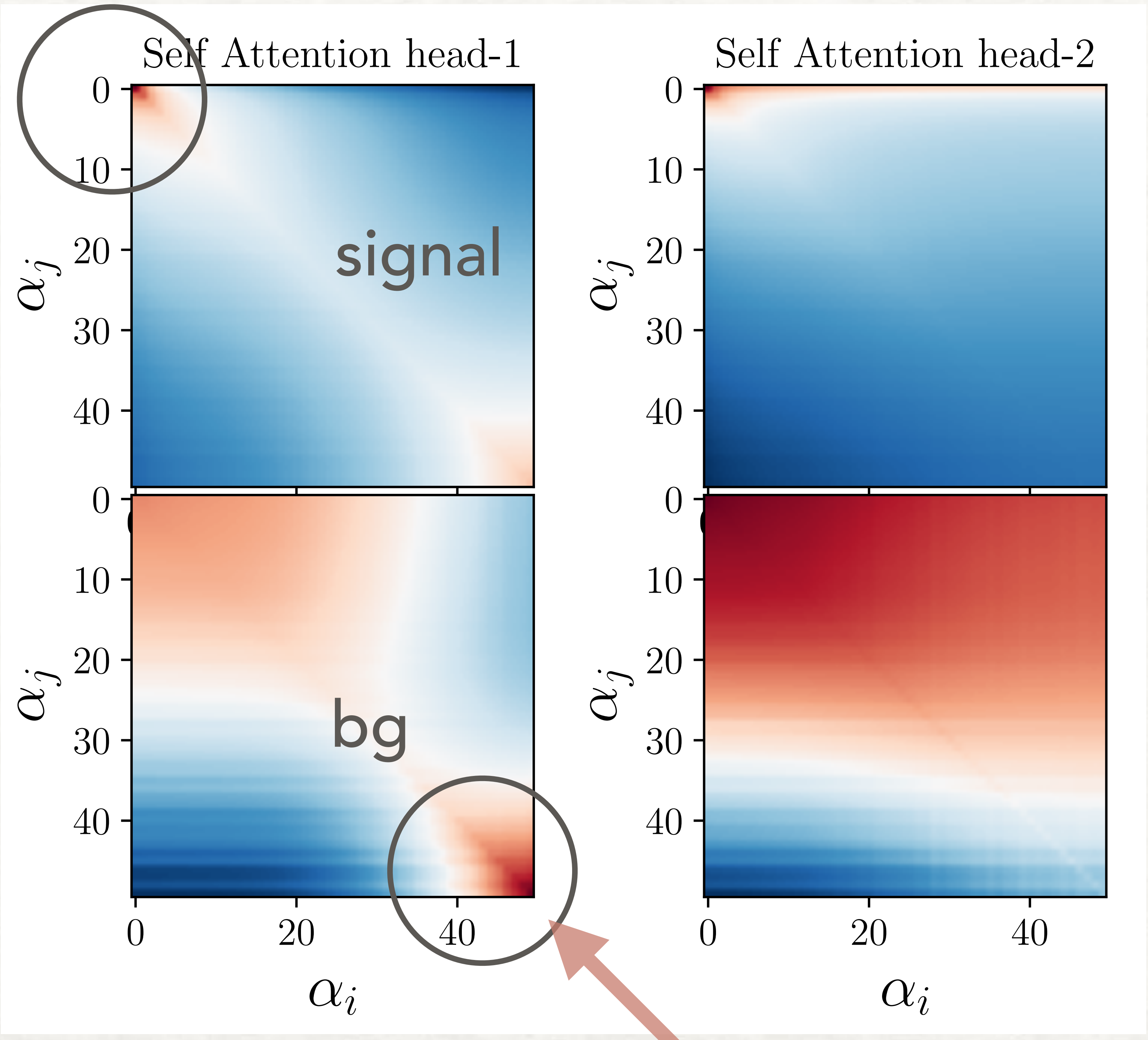
1706.03762 Vaswani et all “Attention is all you need

EX. SELF AND CROSS-ATTENTION MAP

self attention map

axis: odering of modified particles

First few "particle" token express
Higgs nature efficiently

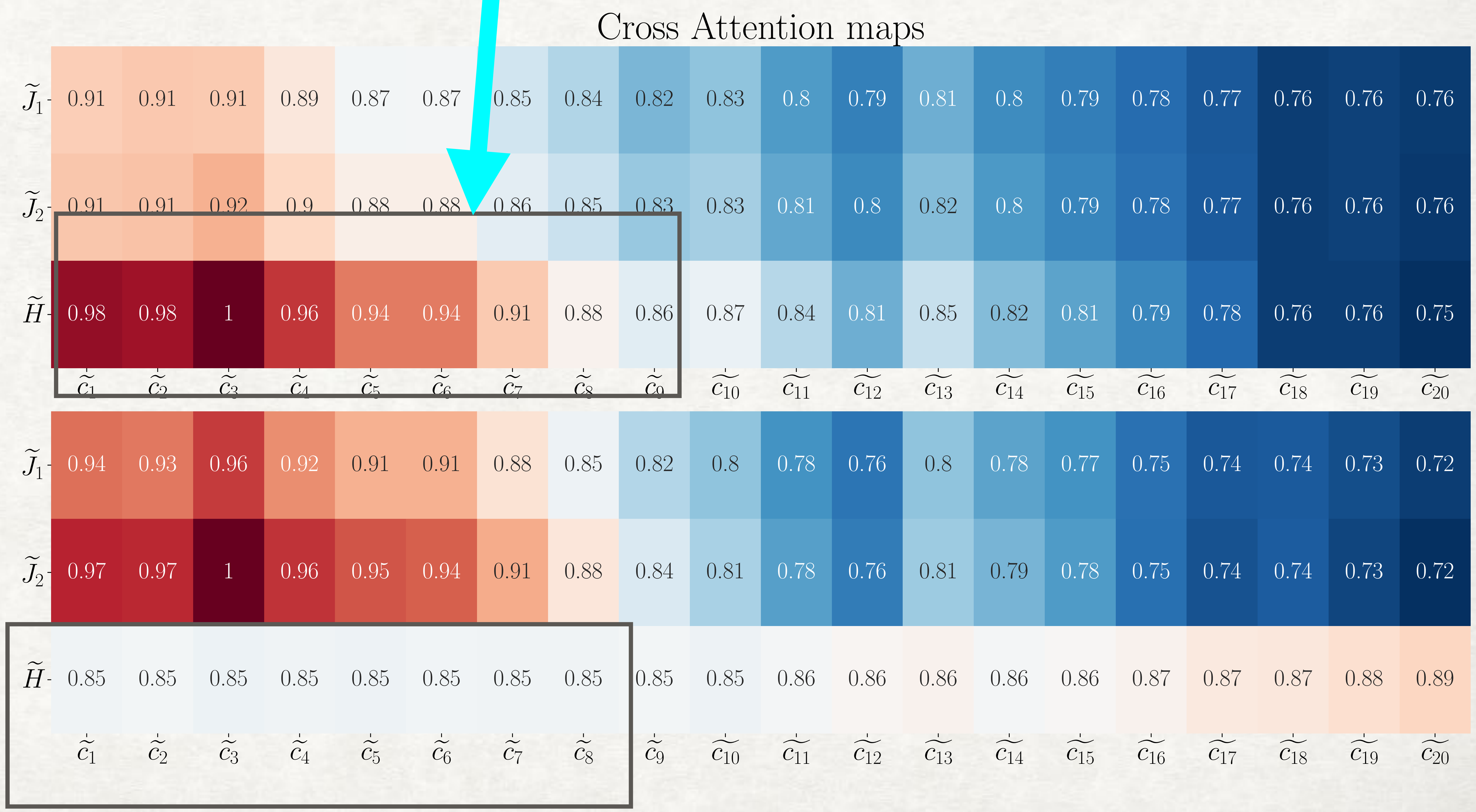


Cross attention map:Particle in the jet (50)
and parent particle (3)

sum of fatjet momenta capture signal

Signal

BG



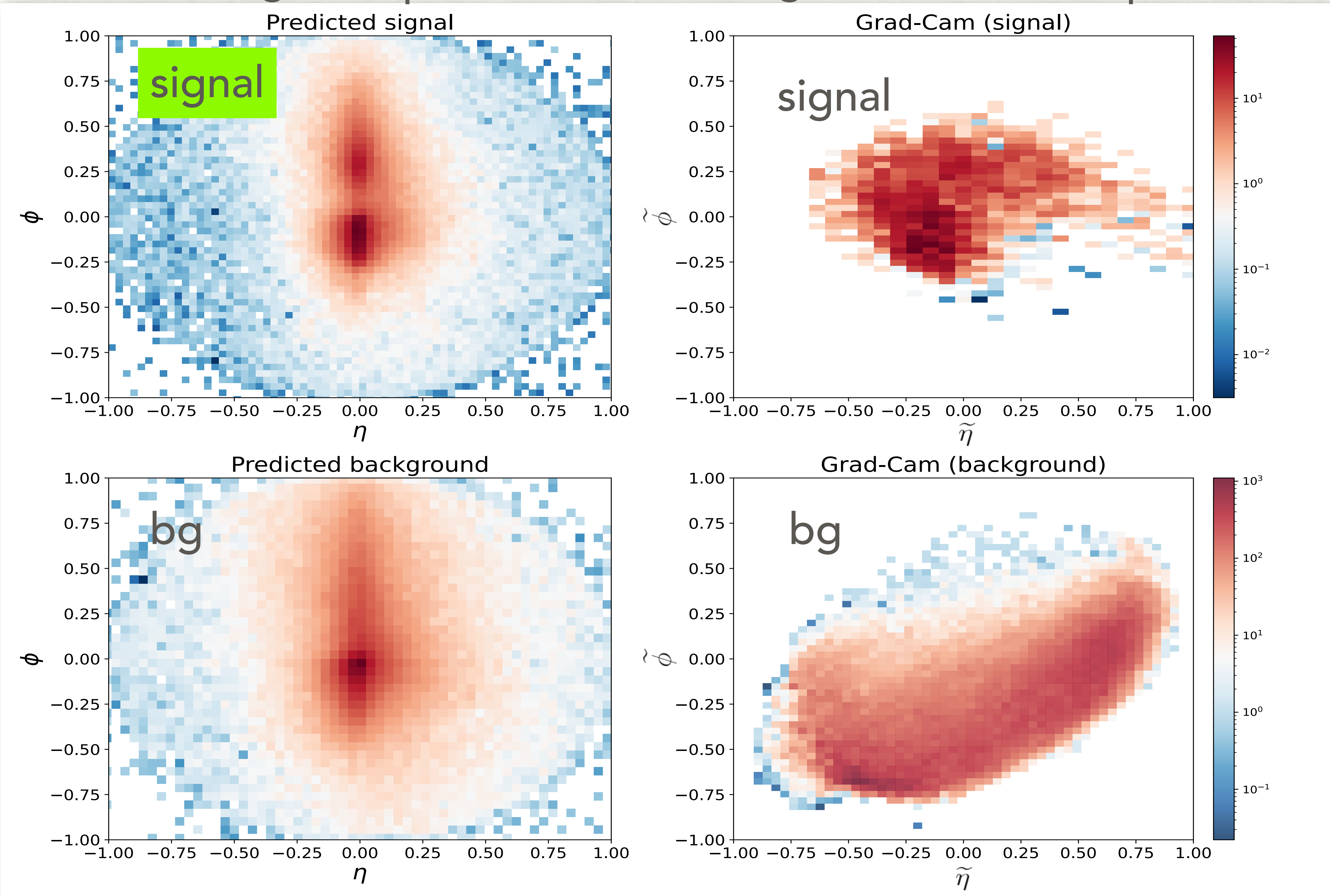
maybe number of averaged particles are different

GRAD-CAM (1610.02391)

- Output of last attension layers (some correlation with original inputs)

5000 signal events

Original inputs grad-cam heatmap



Y : class score

F:output from last attention layer

$\tilde{\eta}, \tilde{\phi}$ transformed corrdinate

$$\alpha_k(\widetilde{\eta}, \widetilde{\phi}) = \frac{1}{Z} \sum \frac{\partial Y_c}{\partial F_k(\widetilde{\eta}, \widetilde{\phi}, \widetilde{p_T})}$$

$$\text{Grad-CAM}(\widetilde{\eta}, \widetilde{\phi}) = \frac{1}{k} \sum_k \alpha_k(\widetilde{\eta}, \widetilde{\phi}) F_k(\widetilde{\eta}, \widetilde{\phi}, \widetilde{p_T})$$

Still see some connection between particle location and transformed coordinates.

Inference vs Attention depth

TAKEAWAYS

- use "cross attention" when you combine the “high scale information” to the “low energy scale”, because cross attention layer gives extra emphasis to the information linked to the high energy kinematics.
- skip connection and Interpretation : Skip connection helps to maintain some connection to the inputs
- More Physics: Heavy particles decay into colored particles (discovery, spin, color structure?) Cross attention network probably more useful to resolve correlation of jet structures.
- Result looks very good to me and I am still worrying about bugs…

NEED TO BE IMPROVED?

- Current GPU requirement: 2 x NVIDIA RTX A6000 (48GB) with 80% and 30% utilization in tensor flow mirror strategy. 96% consumption /card 20min/training.

- reducing computational cost/ Increase Interpretability Campaign :

  - replace "jet substructure part" to something else (keeping cross attention structure:this part is generic) This should also reduce variance in training

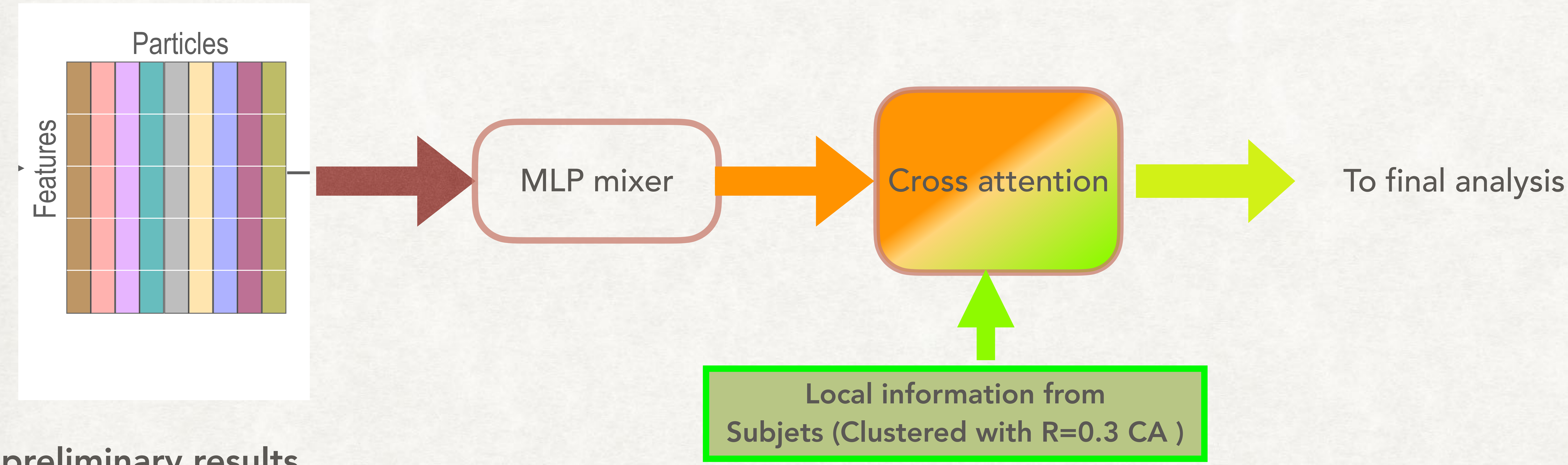
1.transformer for jet substructure → MLP mixer +sujets. (Ahmed Hammad and M.N. in progress)

2. Reducing sparsity using aggregated HL inputs arXiv 2312.11760[hep-ph] "Modulated Network for HL variables" Amon Furuichi(Nagoya), Sung Hak Lim(Rutgers) , M.N

  - are they robust for color connection? transformer may still be useful.

Transformer → MLP-mixer with cross attention (Ahmed Hammad and MN)

Replace jet classification of transformer to subjet X'_{ij} and MLP mixer with cross attention



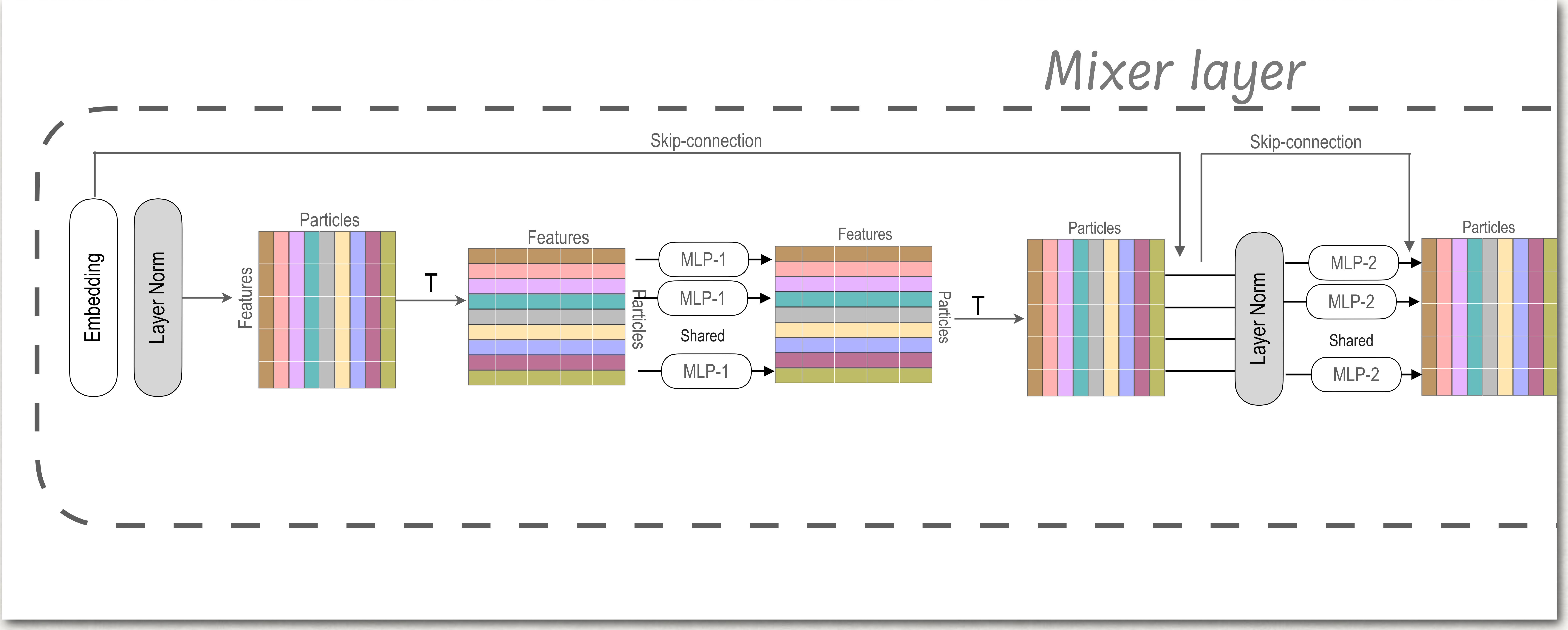
preliminary results

AUC -Transformer = 0.9859 AUC -Mixer = 0.9850	Parameters- Transformer = 1.7M Parameters- Mixer = 94K	Time per epoch- Transformer = 4.2K s Time per epoch- Mixer = 70 s

distribution of TopLandscape community data set
(I do not like using it, because no preselection in it and not good in proving difference)

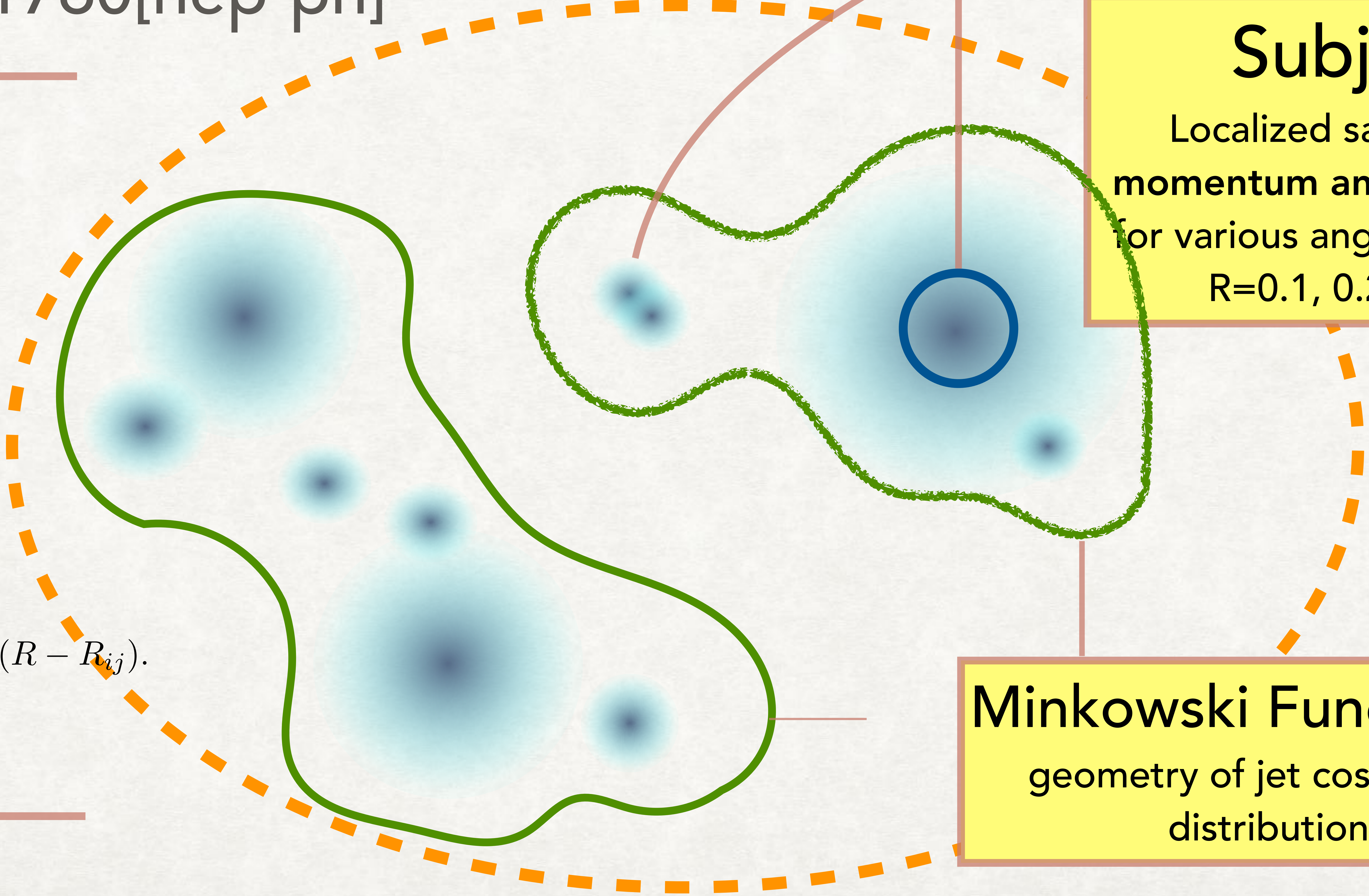
MLP MIXER

The mixer layer has two MLP that mix both features and Particle tokens (similar to the transformer) which allow for fast extraction of the global features of the event. Local information is extracted from the subjects via Cross-attention layer.



2. JET High Level variables
2312.11760[hep-ph]

pt distribution of constituents



Subjet
Localized sampling
momentum and counting
for various angular sccale
R=0.1, 0.2, 0.3

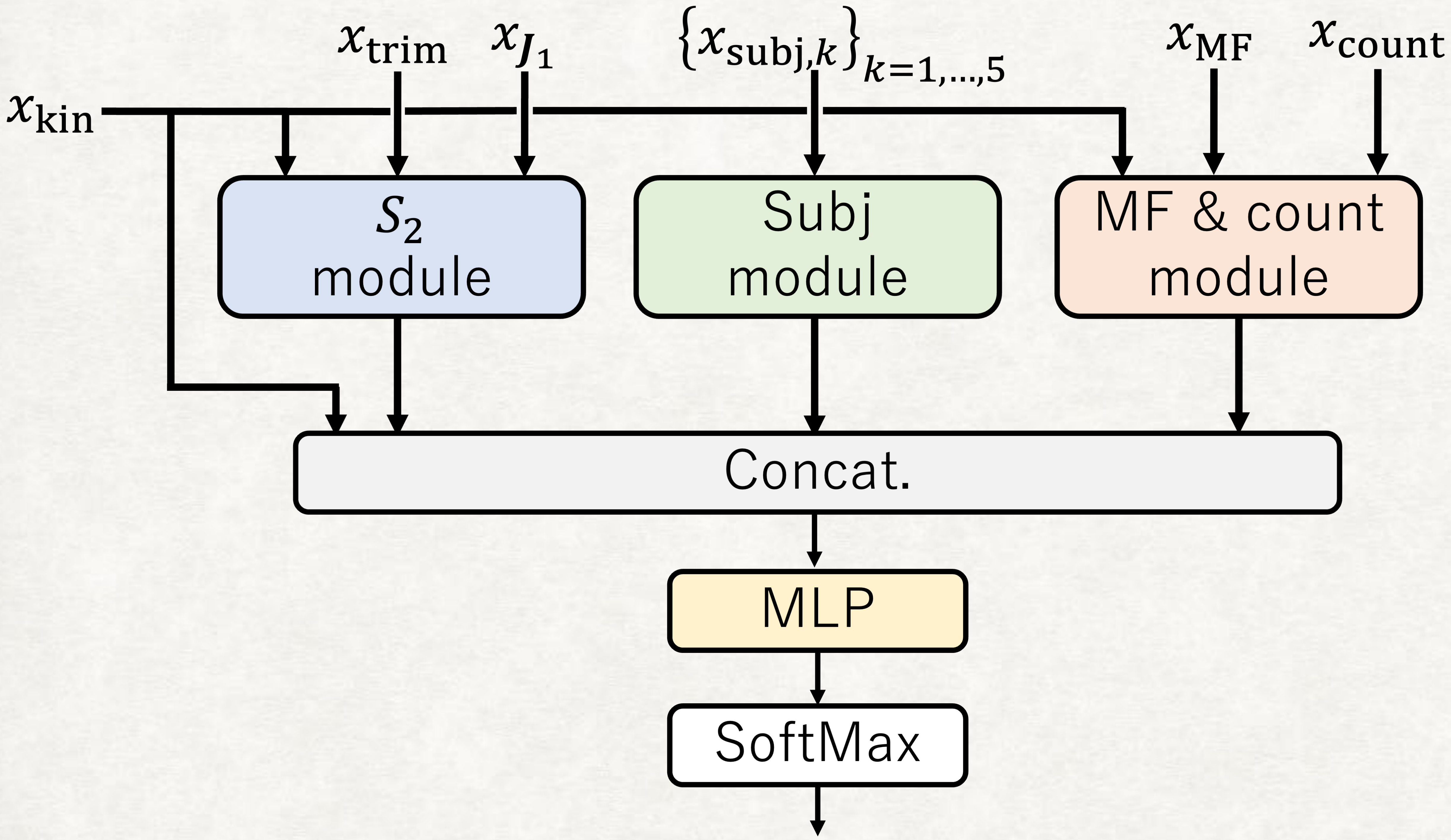
Jet spectrum
two point **Energy correlation**
(unlocalized sampling)

$$S_{2,ab}(R) \stackrel{\text{def}}{=} \sum_{i\in a}\sum_{j\in b} p_{T,i}p_{T,j}\delta(R - R_{ij}).$$

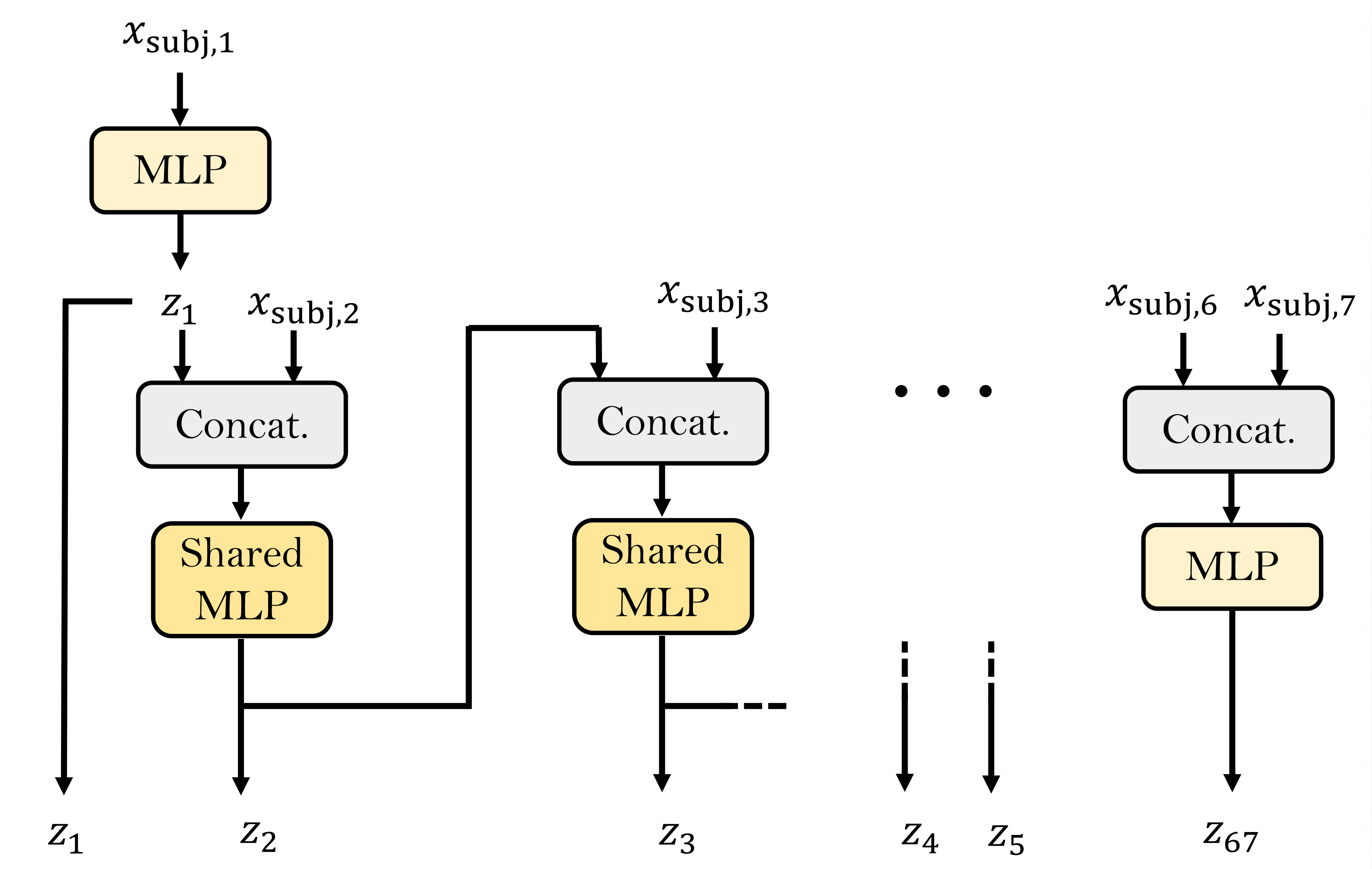
Minkowski Functionals
geometry of jet cosntituent distribution

NETWORK USING HL INPUTS (ANALYSIS MODEL=AM)

easy add and remove



Recluster jet into
Recursive subjet network (pT ordered)

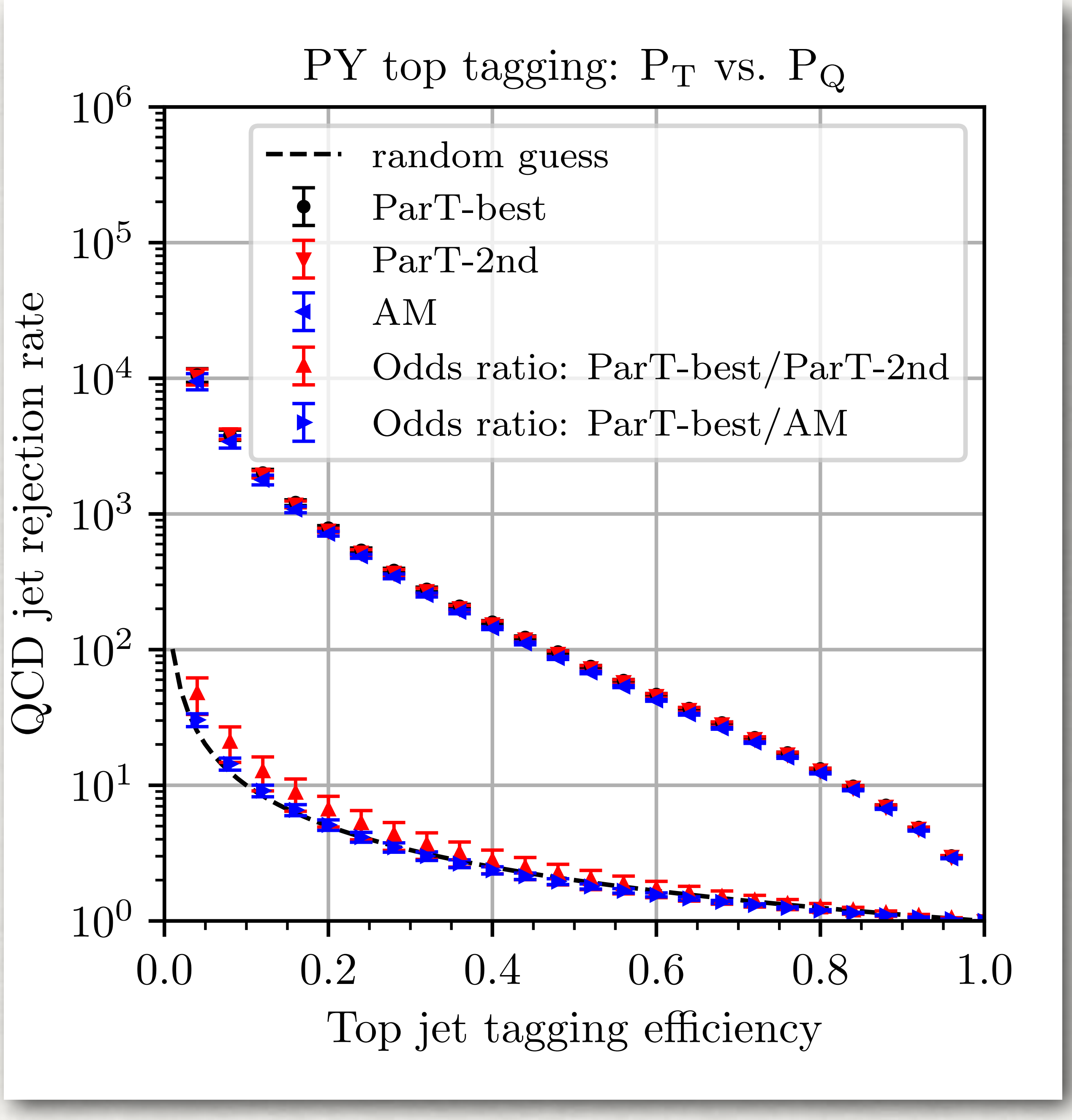


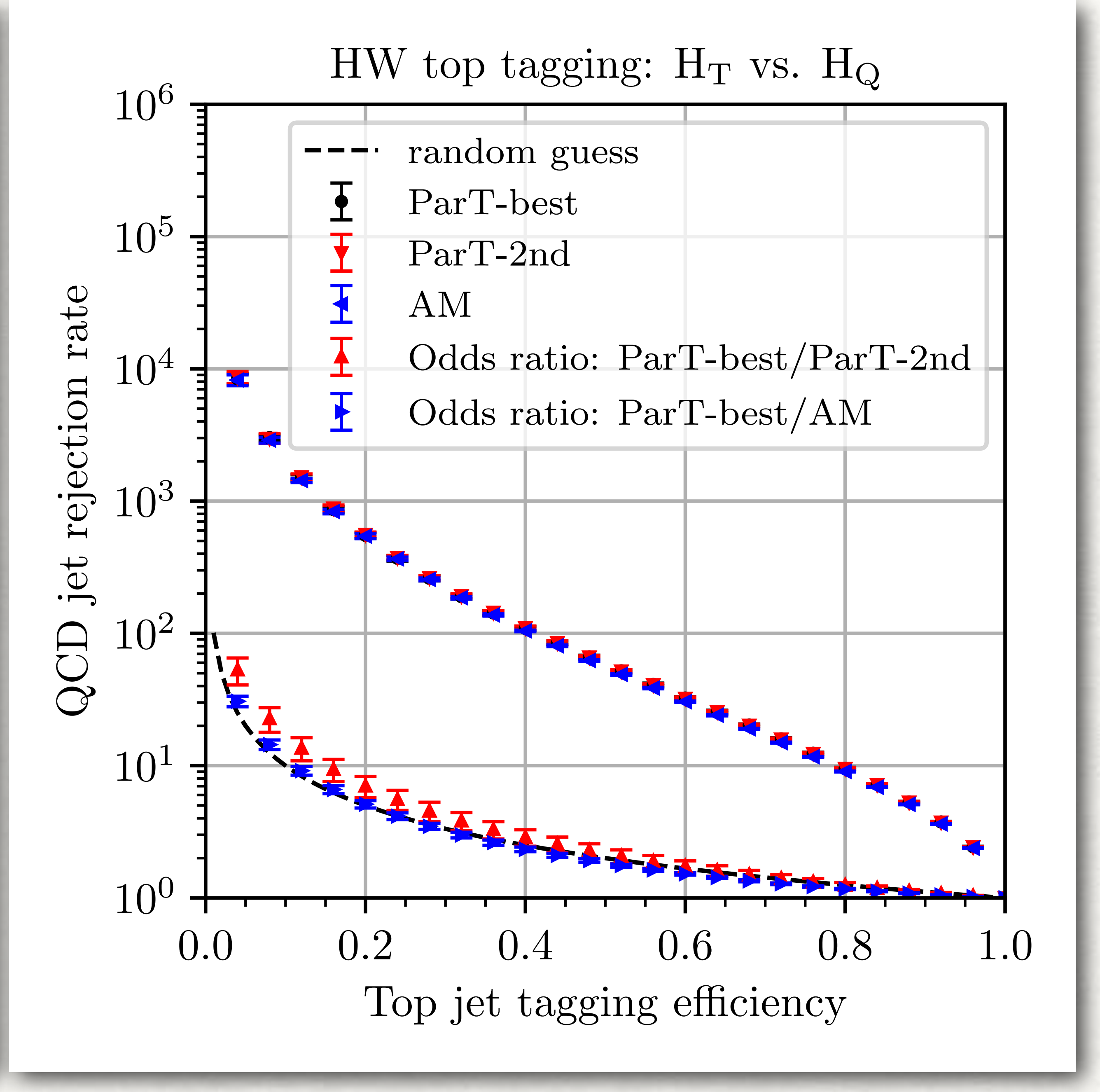
(b) A schematic diagram of subjet recursive module.

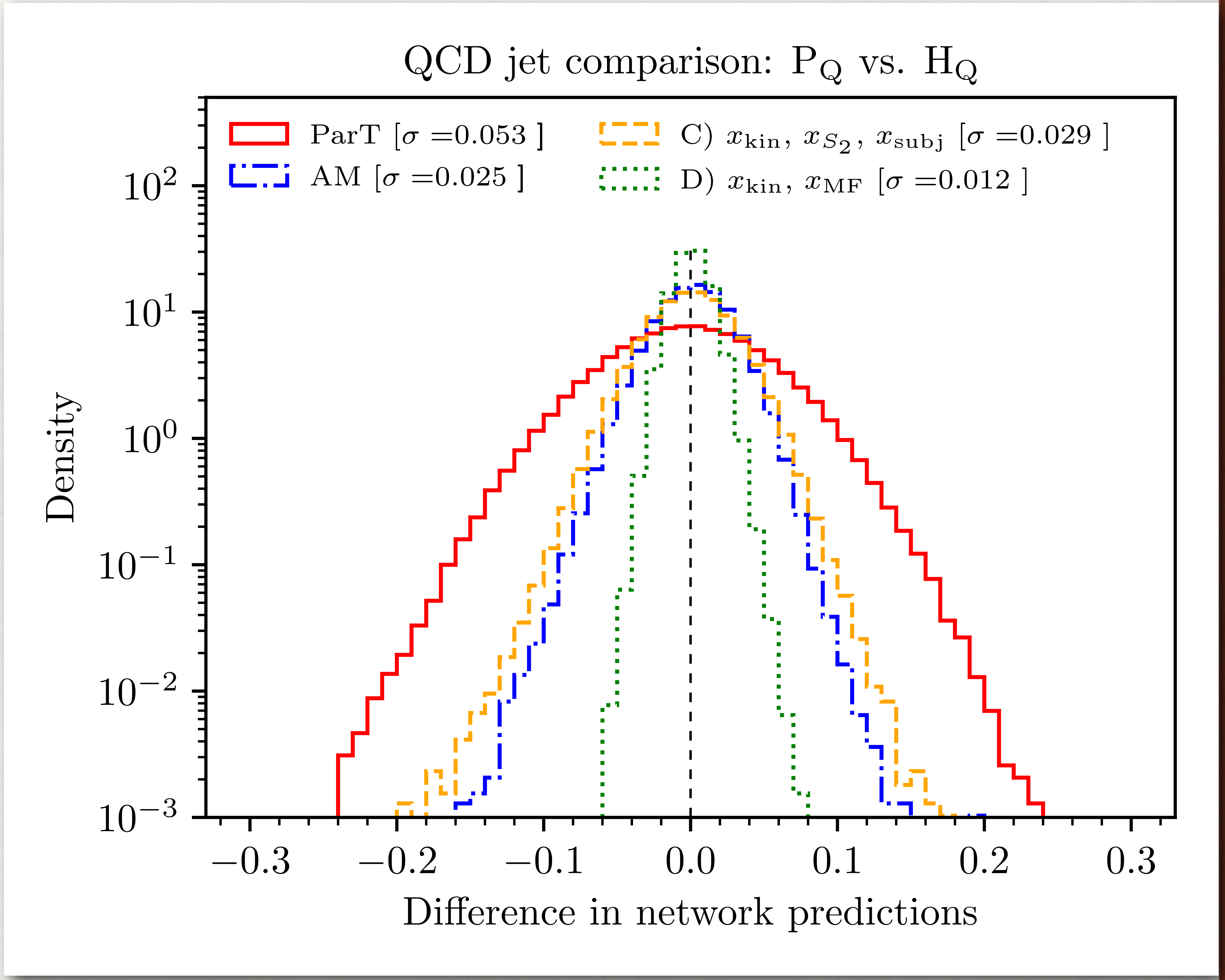
⭐input: subjet with multiple cone size
(R=0.1, 0.2, 0.3) =information of clustering

⭐Shared MLP for 2nd to 5th subjet to reduce paramters

PERFORMANCE AND STABILITY







AM model :**1GB GPU memory** on GeForce 1080Ti GPU(11.3TFLOPS) with 35% GPU utilization. need lots of preprocessing

ParT: **14GB GPU memory** RTX A6000 (38.7TFLOPS) GPU utilization 95%