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Research Training Group Physics of the Heaviest Particles at the LHC

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KAN we improve on HEP classification tasks?

Kolmogorov-Arnold Networks applied to an LHC physics example

arXiv: 2408.02743

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Uncertainties & Interpretability Session

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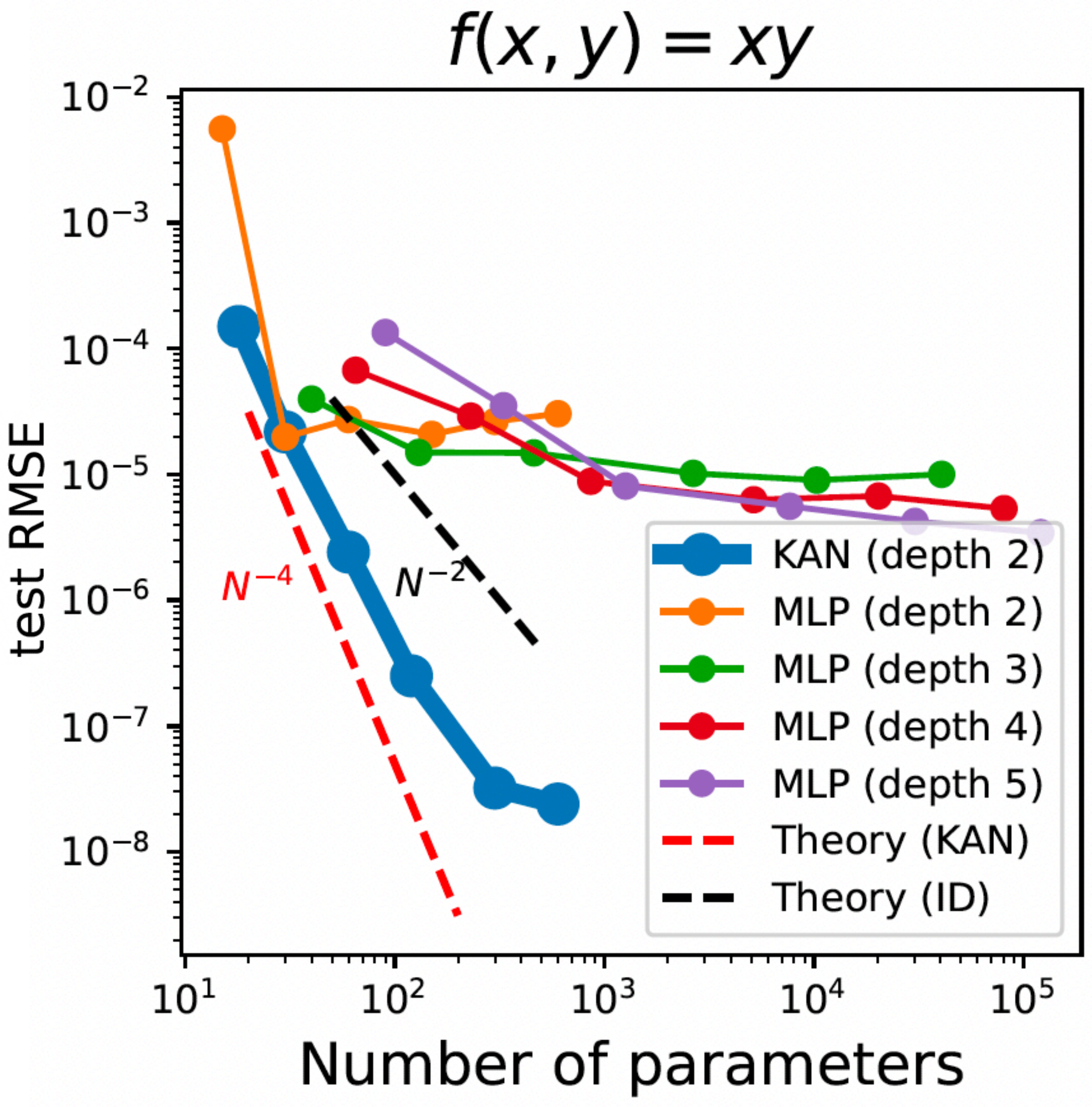
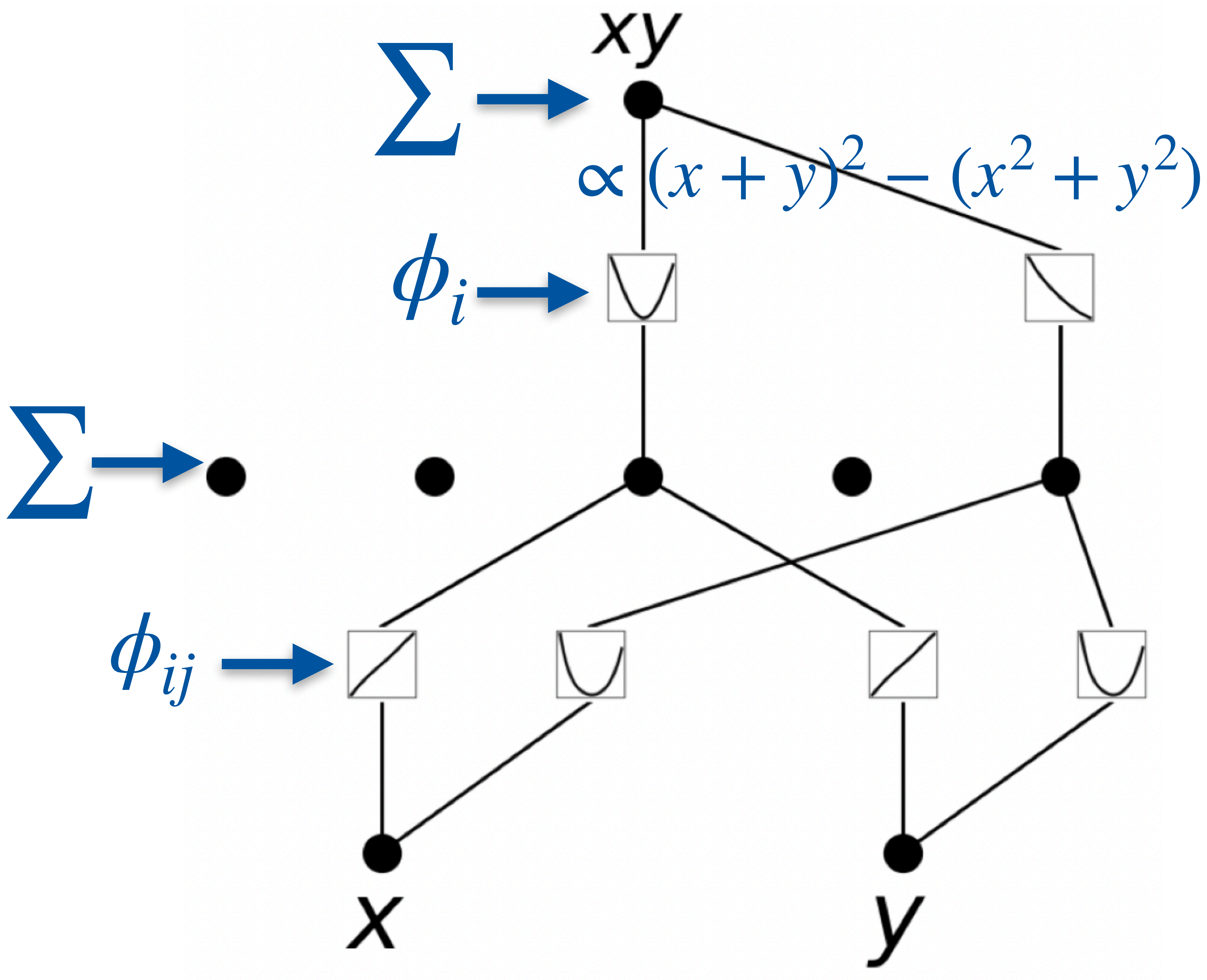
- Kolmogorov-Arnold Networks (KANs) proposed as alternative network architecture
  - Z. Liu et al., 2404.19756
- Advantages over multi-layer perceptrons presented
  - Performance, parameter efficiency and interpretability in multiple tasks
  - Examples provided are rather low dimensional, mathematical datasets
- Efficiency, performance and interpretability are crucial properties in HEP!
  - ➡ Time to explore the potential of KANs here!



Z. Liu et al., 2404.19756

- Inspiration: Kolmogorov-Arnold representation theorem: $f(x_1, x_2, \ldots, x_n) = \sum_{i=1}^{2n+1} \phi_i \left(\sum_{j=1}^{n} \phi_{ij}(x_j) \right)$
  - Continuous multivariate functions can be represented as sum of continuous univariate functions
- Motivates network architecture with learnable univariate functions and sum operation on nodes
- Stacking of "KAN layers" with arbitrary number of nodes proposed in 2404.19756



Z. Liu et al., 2404.19756

	MLPs	KANs
Edges	Linear weights	Learnable activations
Nodes	Fixed activations	Sum

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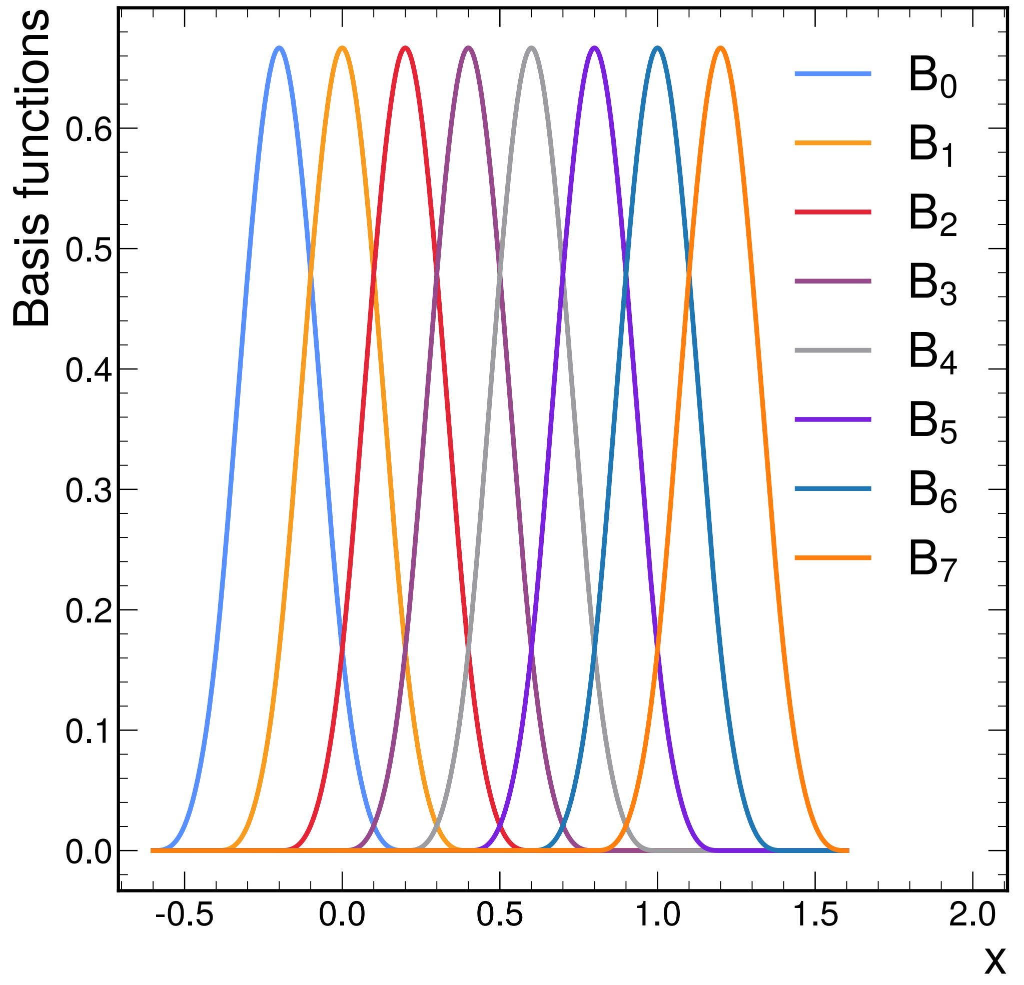
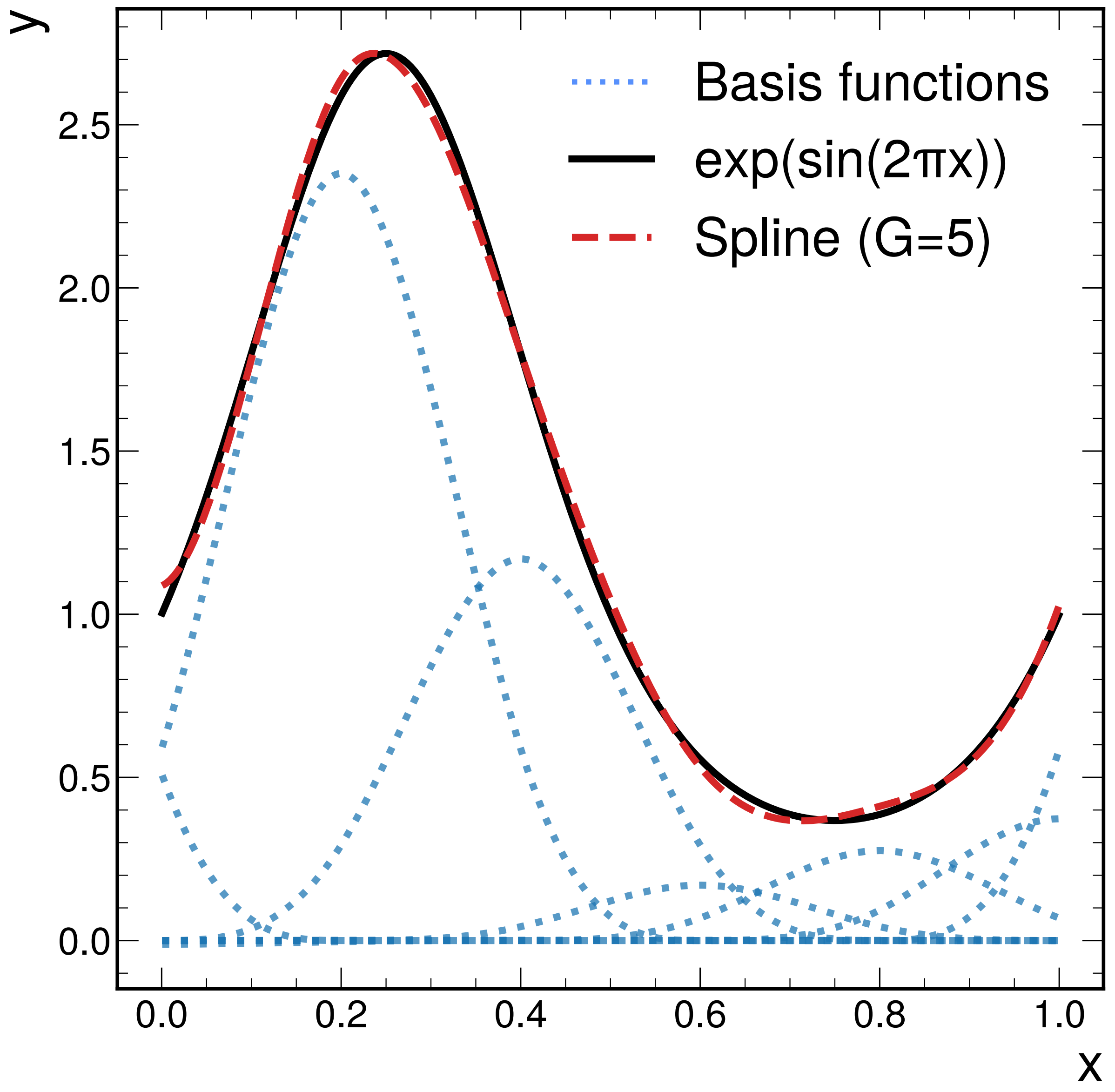
B-splines for learnable activations

- Learnable activation functions can be defined with B-splines
- $\text{activation}(x) = w_1 \cdot \text{SiLU}(x) + w_2 \cdot \sum_{i=0}^{G+k-1} c_i \cdot B_i(x)$
  - w_i, c_i: trainable parameters
  - $B_i(x)$: B-spline basis functions of degree k

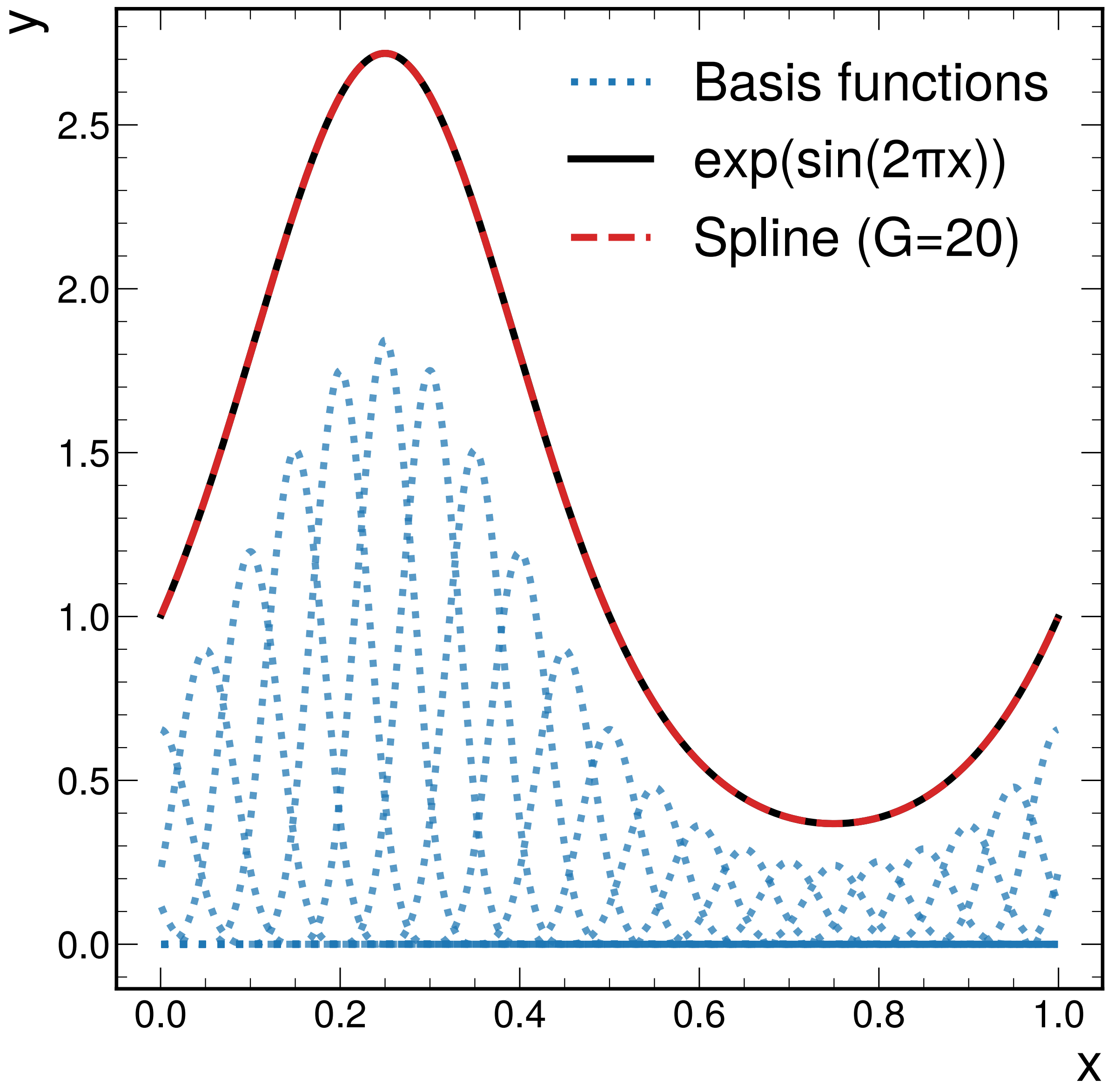
$G = 5,\ k = 3,$
grid range $= (0,1)$



Adapt coefficients c_i
to fit function



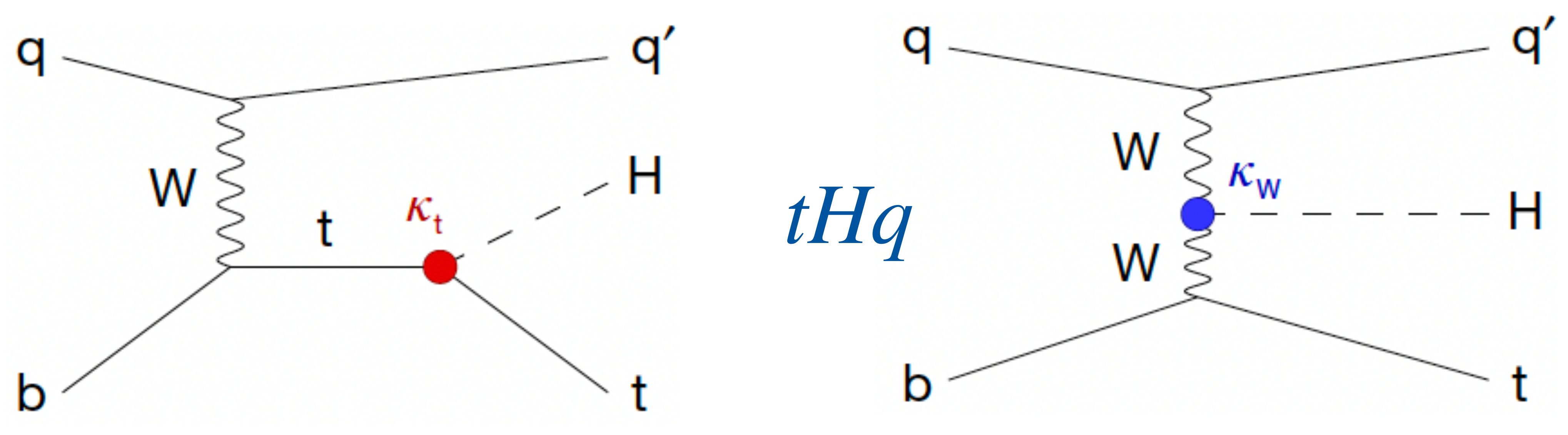
Increase G for
more flexibility



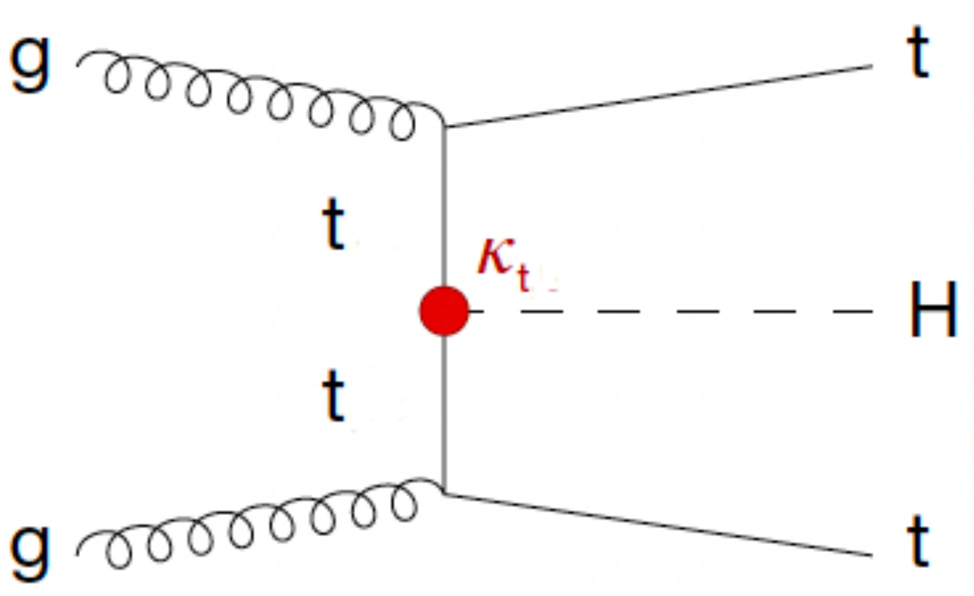
- Grid parameter G regulates number of basis functions, $G + k$ functions used

Dataset

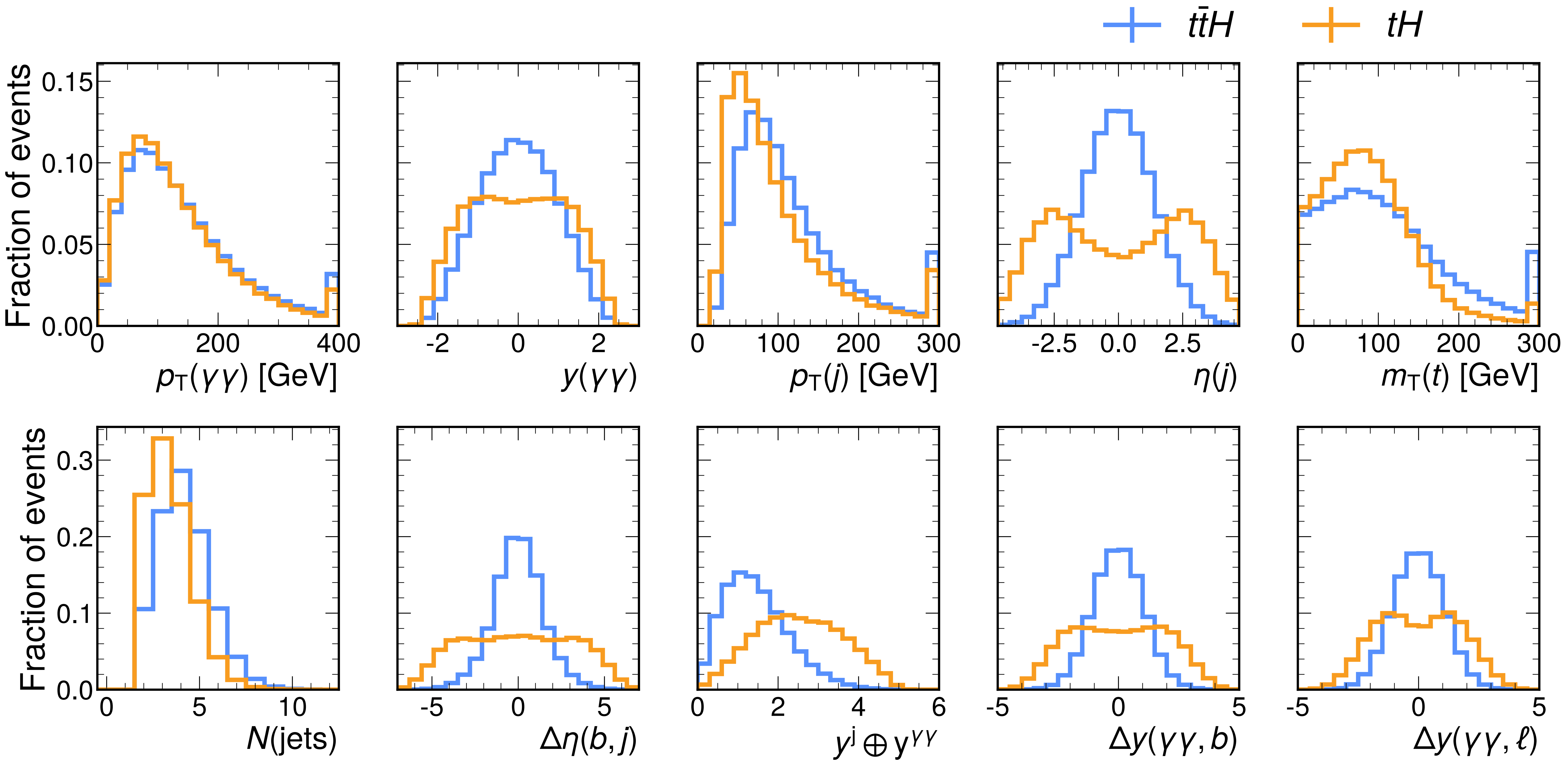
- $t\bar{t}H$ vs. tHq classification in $H \to \gamma\gamma$ decay channel
- MadGraph (LO) + Pythia + Delphes with CMS card
- Typical $H \to \gamma\gamma$ event selection for leptonic channel
- 22 kinematic features constructed



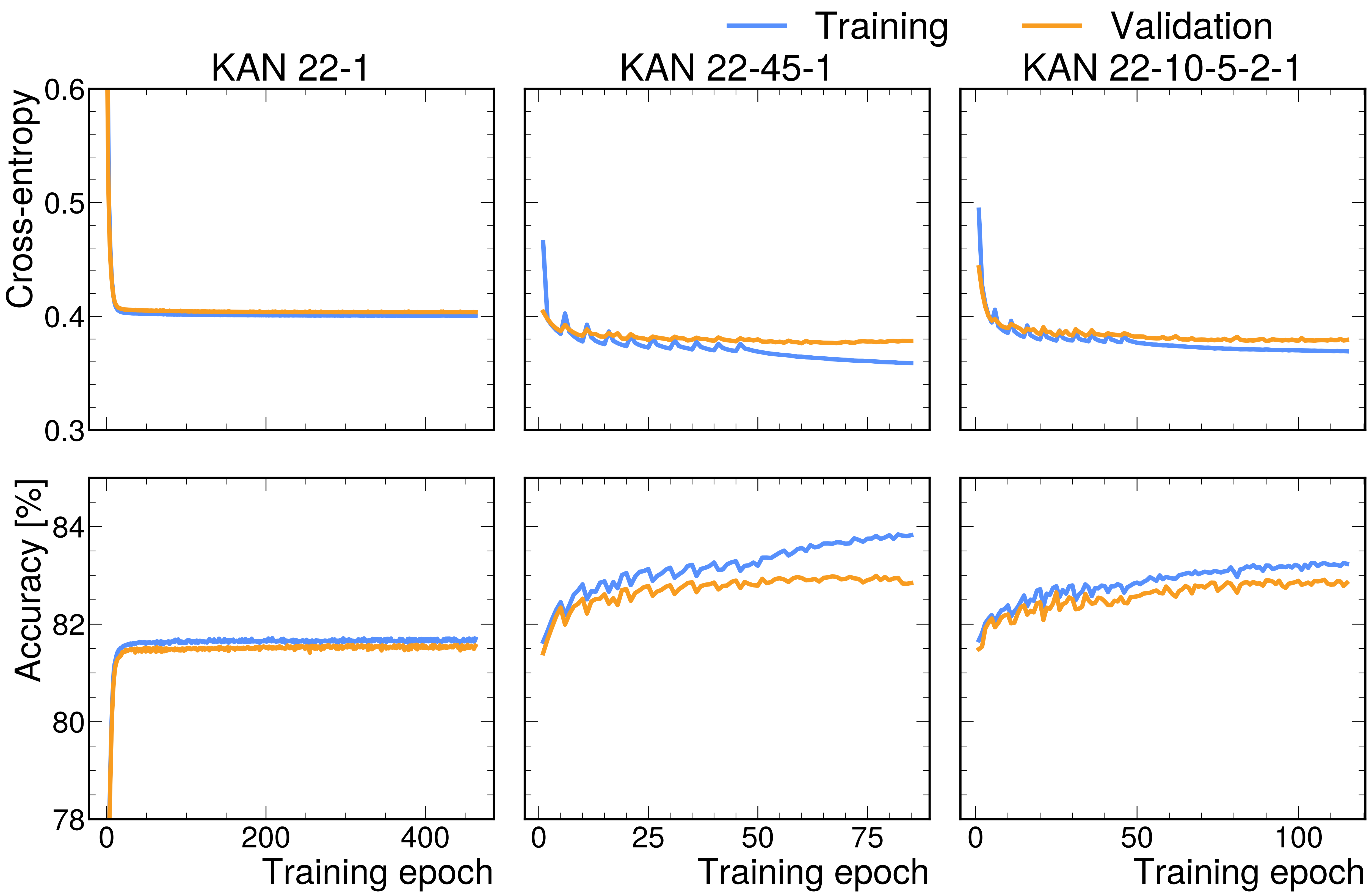
tHq



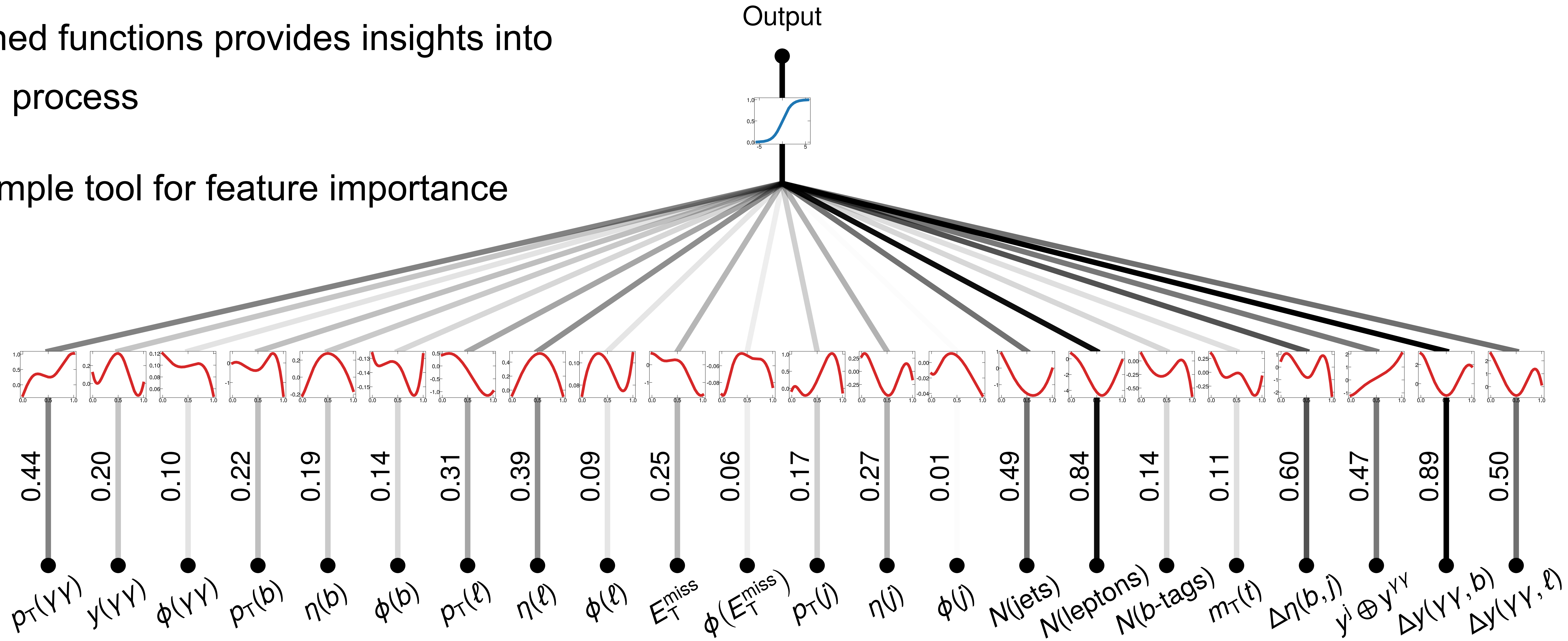
$t\bar{t}H$



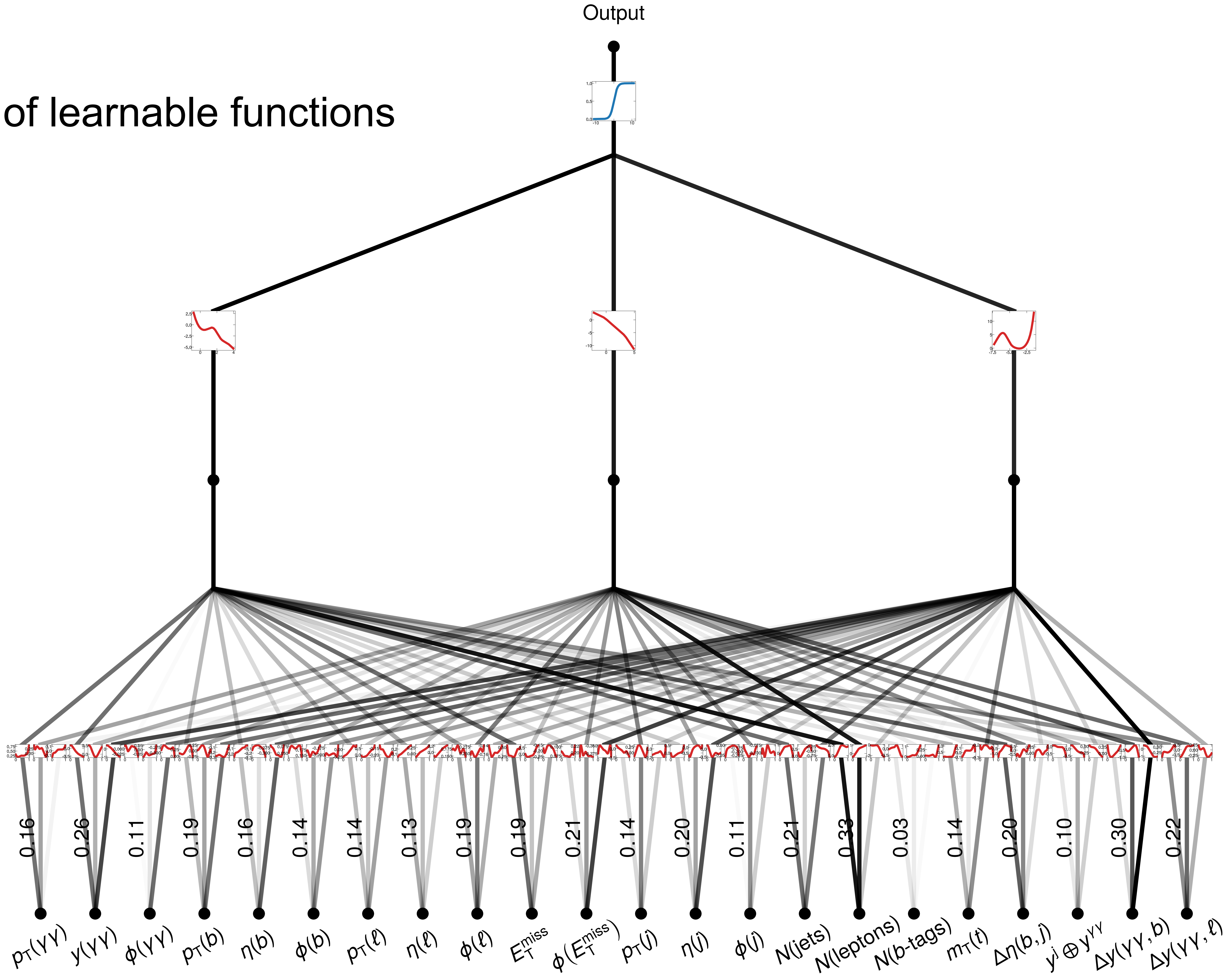
- Using Pykan package for training
- Basic setup for classification task
  - Sigmoid activation of output
  - Cross-entropy loss
  - Adam optimizer
- Stable trainings without much fine-tuning found
- Even single-layer network reaches >81.5% accuracy, two layers needed for better performance (~83%)



- Small models: moderate number of spline functions
  - Here: single-layer KAN (22–1)
- Analysing learned functions provides insights into model decision process
- L_1-norms as simple tool for feature importance

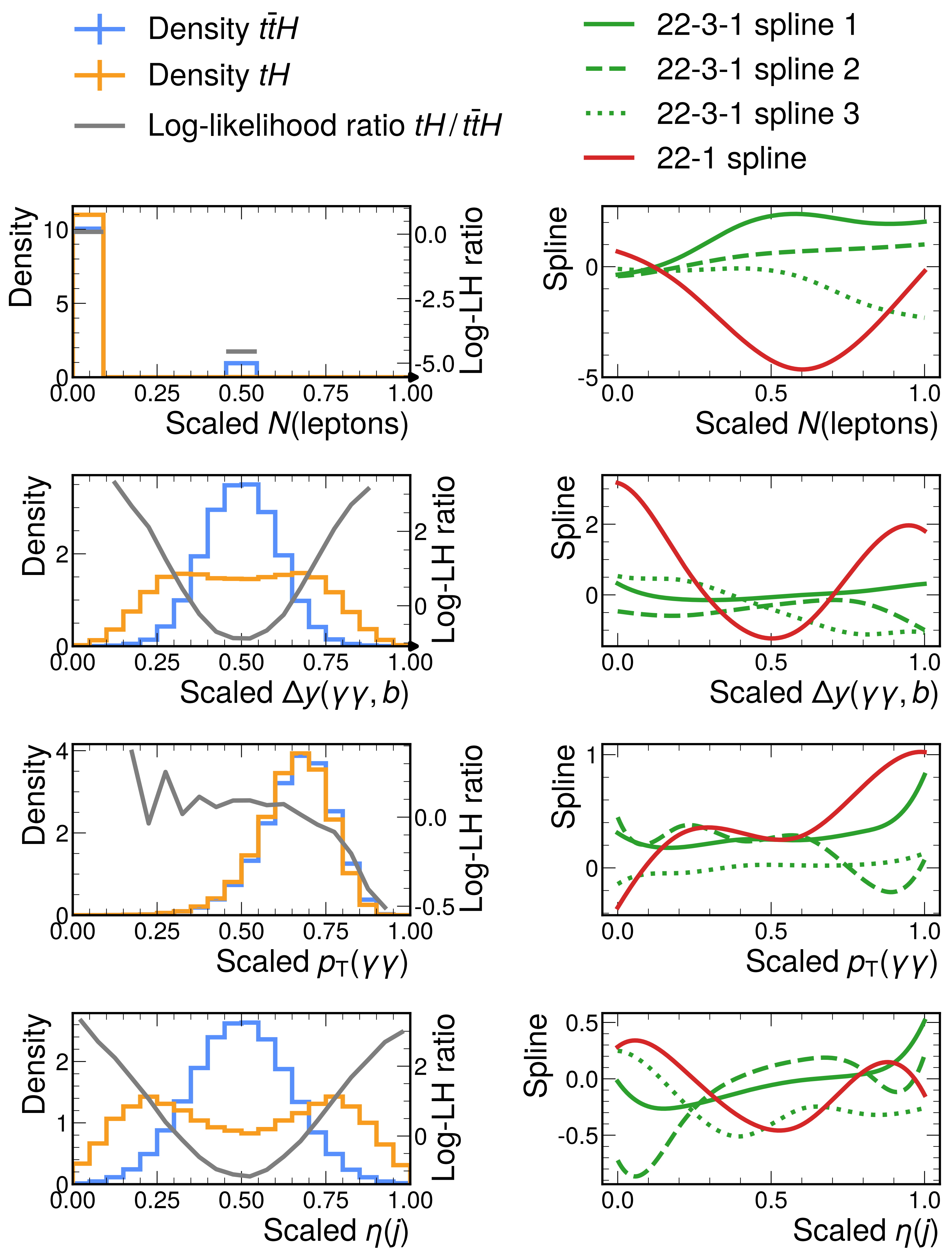


- Deeper / wider models can contain large number of learnable functions
  - E.g. 22–45–1 KAN: > 1000 splines
  - Here: 22–3–1 KAN: 69 splines
- Understanding the reasoning of larger models becomes very difficult

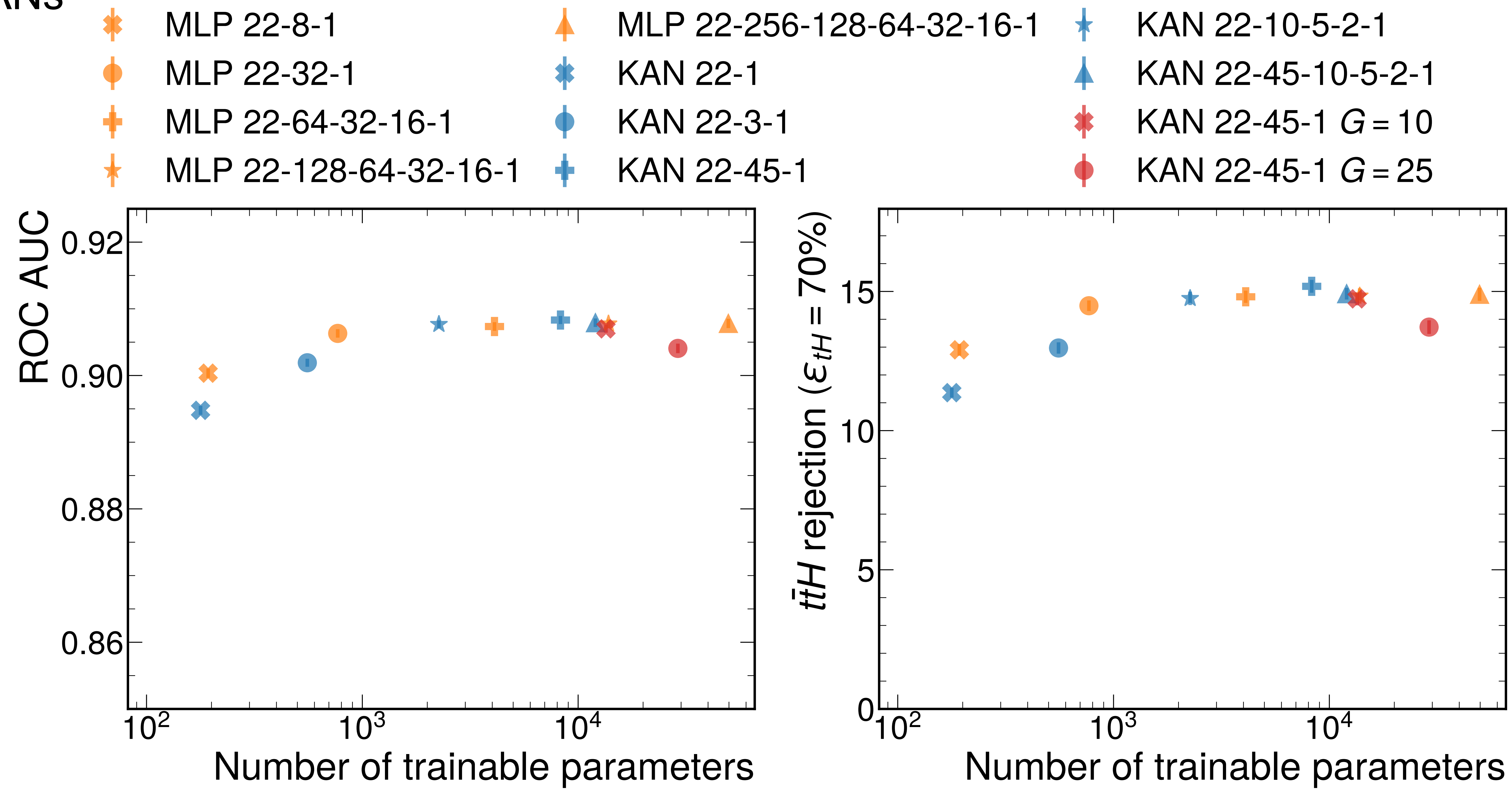


Interpretability: splines

- Patterns can be observed in small models
- Single-layer KAN:
  - One function transforms each input feature
  - Splines often resemble log-likelihood ratio of input features
- Deeper and wider KANs:
  - Many functions act on one input feature
  - More complex representations of input data

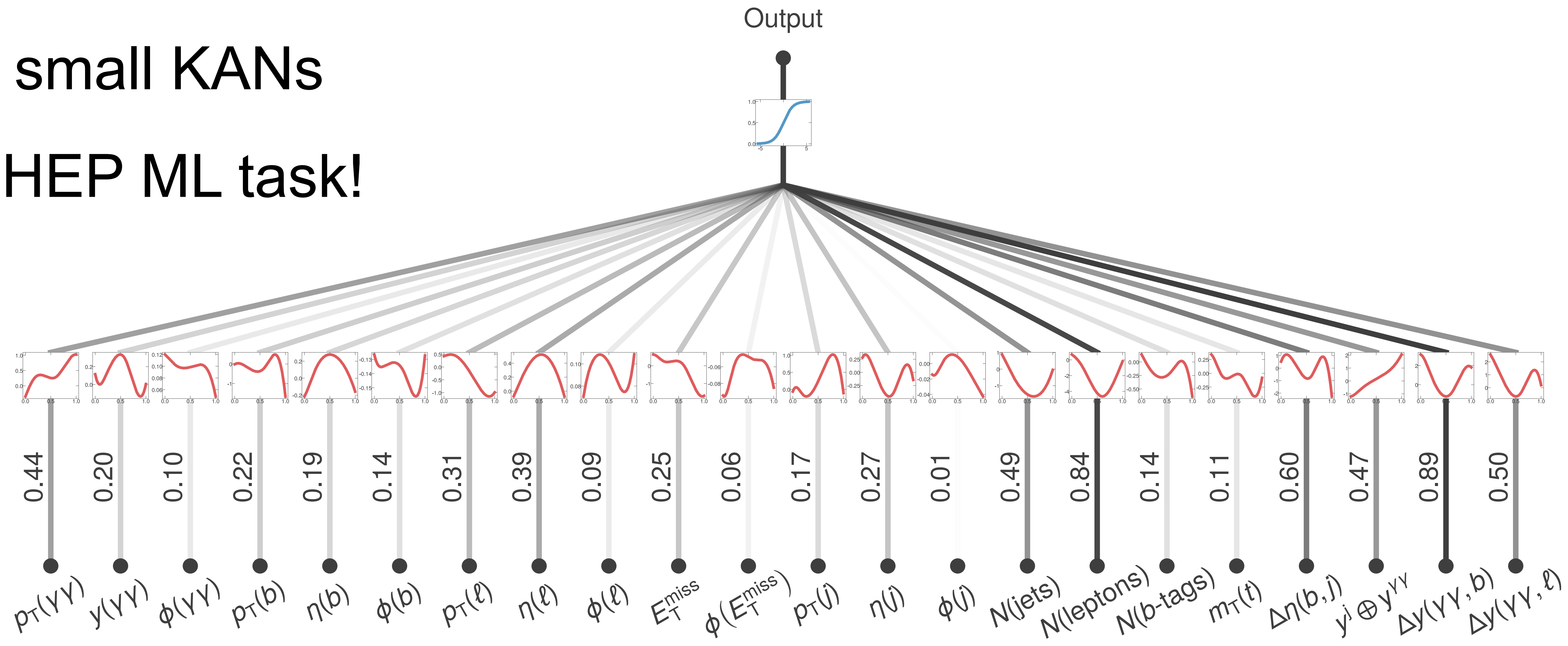


- Studied MLPs and KANs of different architectures for this task
- <1000 trainable parameters: MLPs beat KANs
    - Interpretability of small KANs comes at a cost in performance
- Similar performance for models with more parameters
    - Best tested model was a KAN!



Conclusions

- Applied Kolmogorov-Arnold Networks to high-energy physics for the first time
- Classification of $t\bar{t}H$ & tH events in $H \rightarrow \gamma\gamma$ decay channel
  - Example of typical complexity for binary HEP event classification
- Observed that KANs can achieve similar performance as MLPs, but don't appear more parameter efficient on our dataset
- Advantages in interpretability over MLPs exist for small KANs
  - May be worth to consider KANs for your next HEP ML task!
- Pre-print about our study: [2408.02743]



Backup

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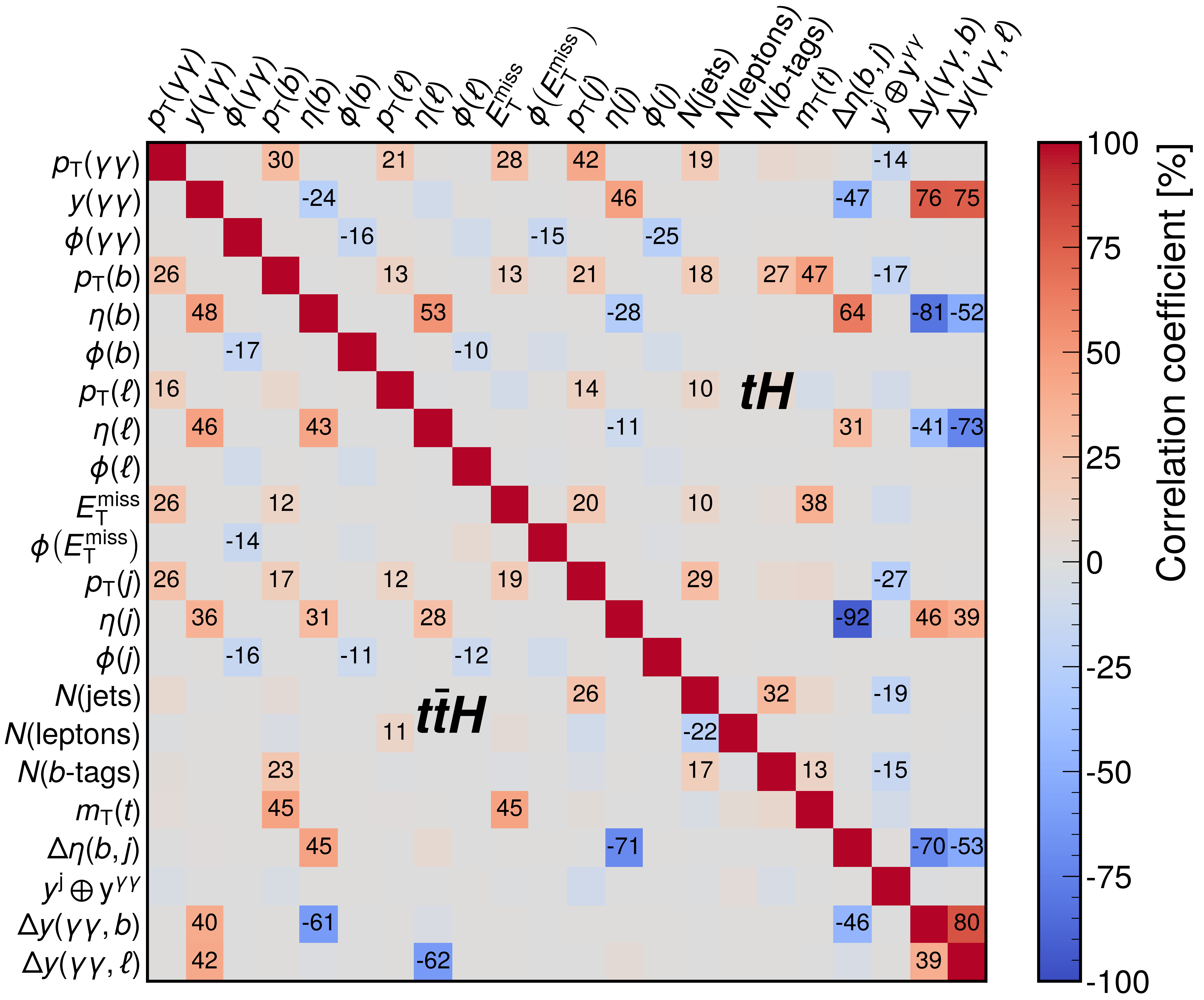
Correlations of features

- Non-trivial correlation pattern
- Significant differences between the two classes



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B-spline basis functions

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➡ Recursive definition with Cox–de Boor formula

- $B_i^0(x) = 1$ if $t_i \leq x < t_{i+1}$; $B_i^0(x) = 0$ otherwise
- For $k > 0$: $B_i^k(x) = \frac{x - t_i}{t_{i+k} - t_i} B_i^{k-1}(x) + \frac{t_{i+k+1} - x}{t_{i+k+1} - t_{i+1}} B_{i+1}^{k-1}(x)$.