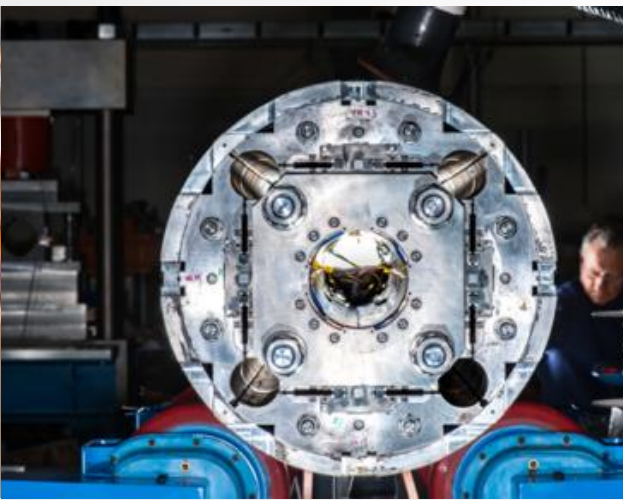




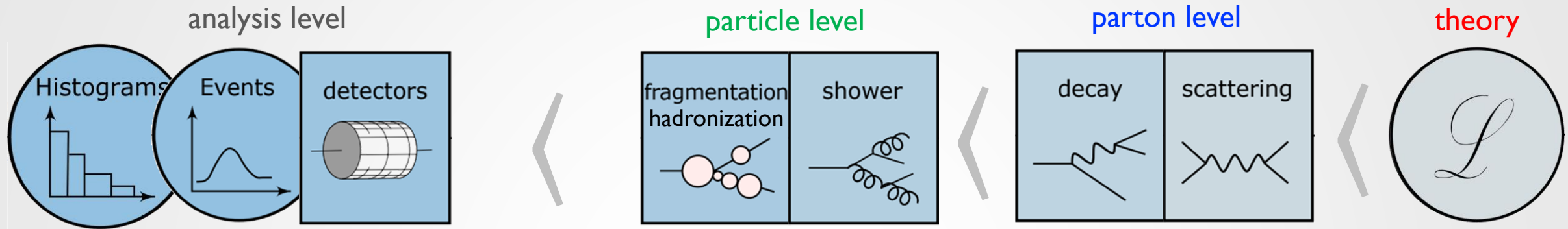
TREE BOOSTING (+NEURAL NETWORKS) FOR EFT ANALYSES

R. Schöfbeck (HEPHY Vienna), Oct.. 24th, 2023, Area 3 meeting



A CONDITIONAL SEQUENCE

adapted from [arXiv:2211.01421](https://arxiv.org/abs/2211.01421)



$$p(x_{\text{det}}|\theta) = \int dz_{\text{ptl}} \int dz_{\text{p}} [\dots] p(x_{\text{det}}|z_{\text{ptl}}) p(z_{\text{ptl}}|z_{\text{p}}) p(z_{\text{p}}|\theta)$$

ML facilitates this inversion by exploiting that simulation samples

$$x_{\text{det}}, z_{\text{ptl}}, z_{\text{p}} \sim p(x_{\text{det}}, z_{\text{ptl}}, z_{\text{p}}|\theta)$$

“Simulation based inference”

1. Generators run in ‘forward mode’
2. Pick up uncertainties

$$p(z_{\text{ptl}}|z_{\text{p}}, \nu_{\text{th.}})$$

$$p(x_{\text{det}}|z_{\text{ptl}}, \nu_{\text{exp.}})$$

$$\frac{1}{\sigma_{\theta}} \frac{d\sigma_{\theta}}{dz_{\text{p}}} = p(z_{\text{p}}|\theta)$$

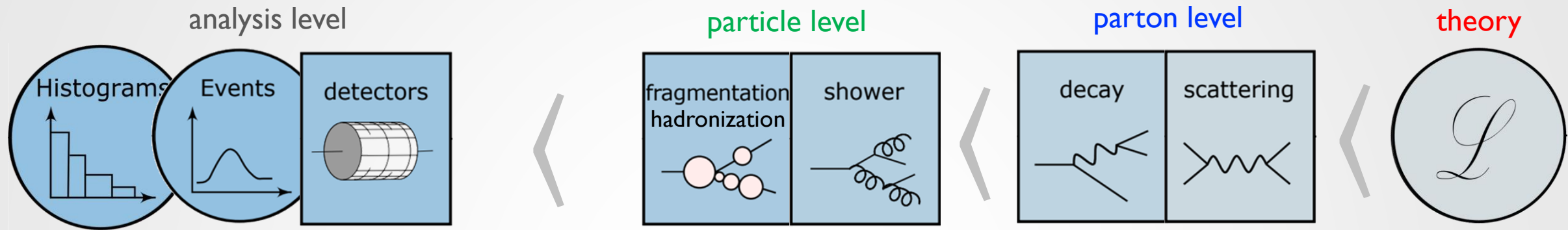
parton-level
differential cross section
~ pdf

~~$$p(\theta)$$~~

θ NOT
stochastic;
Frequentist

THE LIKELIHOOD RATIO TRICK

adapted from [arXiv:2211.01421](https://arxiv.org/abs/2211.01421)



Event classification $\theta \rightarrow \text{isSig} \in \{0,1\}$

$$L = \langle f(x)^2 \rangle_{\text{isSig}=1} + \langle (1 - f(x))^2 \rangle_{\text{isSig}=0} = \sum_{\text{isSig}} \int dx \dots$$

$$f^*(x) = \frac{1}{1 + \frac{p(x|\text{isSig}=1)}{p(x|\text{isSig}=0)}}$$

Learn LR by classification;
“Likelihood ratio trick”
achieve NP optimality (for x-sec)

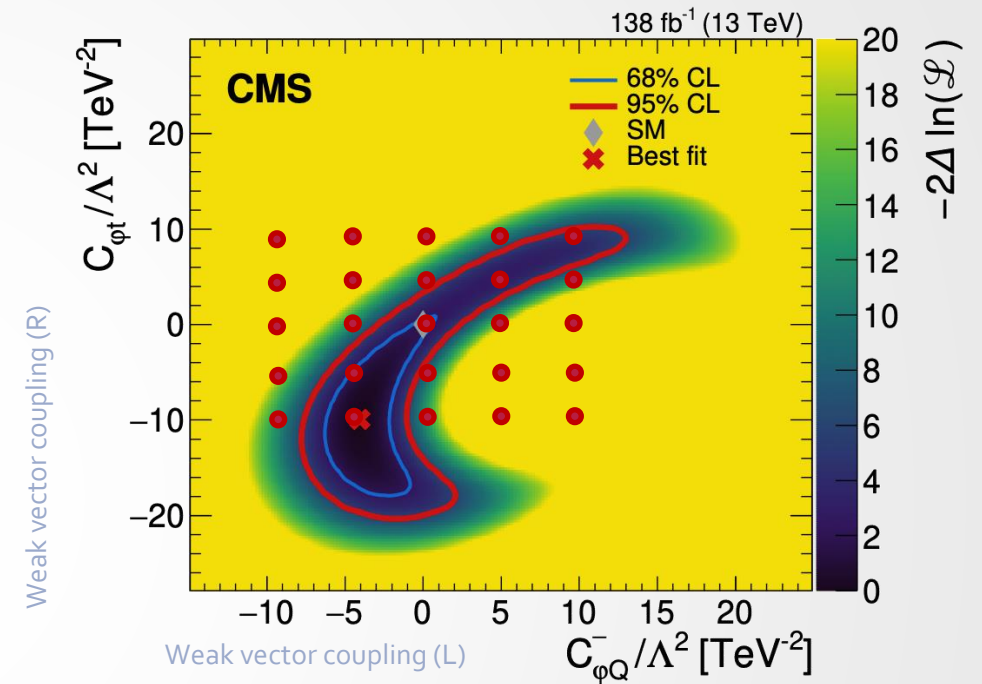
CAN WE JUST LEARN EFT EFFECTS "ON AVERAGE"?

$$L = \sum_{\theta \in \mathcal{B}} \int d\mathbf{x} \left(p(\mathbf{x}|\theta) \hat{f}(\mathbf{x})^2 + p(\mathbf{x}|\text{SM})(1 - \hat{f}(\mathbf{x}))^2 \right)$$

θ - ignorant

mixing signals & case dependent mixes

$$f^*(\mathbf{x}) = \frac{1}{1 + r_{\mathcal{B}}(\mathbf{x})} \quad r_{\mathcal{B}}(\mathbf{x}) = \frac{\frac{1}{|\mathcal{B}|} \sum_{\theta \in \mathcal{B}} p(\mathbf{x}|\theta)}{p(\mathbf{x}|\text{SM})}$$



[TOP-21-001]

- We can try to learn EFT effects "on average"
- Sending 'mixed signals' to the loss function
 - Averages the training data set - suboptimal when linear effects dominate
 - Classifier does not reflect knowledge on the θ -dependence
- 1. Back to the drawing board & inject θ polynomial SMEFT dependence in estimator.
- 2. Exploit the fact that SMEFT predictions can (optionally) be weighted: Only need one training data set

EXPLOITING SMEFT REWEIGHTING

$$L = \sum_{\theta \in \mathcal{B}} \left(\langle \hat{f}(x; \theta)^2 \rangle_{\theta} + \langle (1 - \hat{f}(x; \theta))^2 \rangle_{\text{SM}} \right)$$

θ -aware
EFT sample
SM sample

We start with SM and **BSM** samples

$$= \sum_{\theta \in \mathcal{B}} \int dx dz \left(p(x, z | \theta) \hat{f}(x; \theta)^2 + p(x, z | \text{SM}) (1 - \hat{f}(x; \theta))^2 \right)$$

Let's write this under one integral
z ... latent space

$$= \sum_{\theta \in \mathcal{B}} \int dx dz p(x, z | \text{SM}) \left(r(x, z | \theta) \hat{f}(x; \theta)^2 + (1 - \hat{f}(x; \theta))^2 \right)$$

SM sample
↑
"joint" likelihood ratio

... and use just one sample
& joint likelihood ratio

$$r = \frac{p(x_{\text{det}}, \dots, z_{\text{ptl}}, \dots, z_{\text{p}} | \theta)}{p(x_{\text{det}}, \dots, z_{\text{ptl}}, \dots, z_{\text{p}} | \text{SM})} = \frac{p(x_{\text{det}} | z_{\text{ptl}}) \cdots p(z_{\text{ptl}} | z_{\text{p}}) \cdots p(z_{\text{p}} | \theta)}{p(x_{\text{det}} | z_{\text{ptl}}) \cdots p(z_{\text{ptl}} | z_{\text{p}}) \cdots p(z_{\text{p}} | \text{SM})} = \frac{p(z_{\text{p}} | \theta)}{p(z_{\text{p}} | \text{SM})} \sim \frac{|\mathcal{M}(z_{\text{p}}, \theta)|^2}{|\mathcal{M}(z_{\text{p}}, \text{SM})|^2} = w_i(\theta)$$

Change in likelihood of simulated observation x
with latent "history" z going from "SM" to θ

staged simulation in forward mode:
Intractable factors cancel

re-calculable
theory prediction

weighted
simulation

PARAMETRIZED CLASSIFIERS

$$L = \sum_{\theta \in \mathcal{B}} \int dx dz p(x, z | \text{SM}) \left(r(x, z | \theta) \hat{f}(x; \theta)^2 + (1 - \hat{f}(x; \theta))^2 \right)$$

MSE or cross entropy

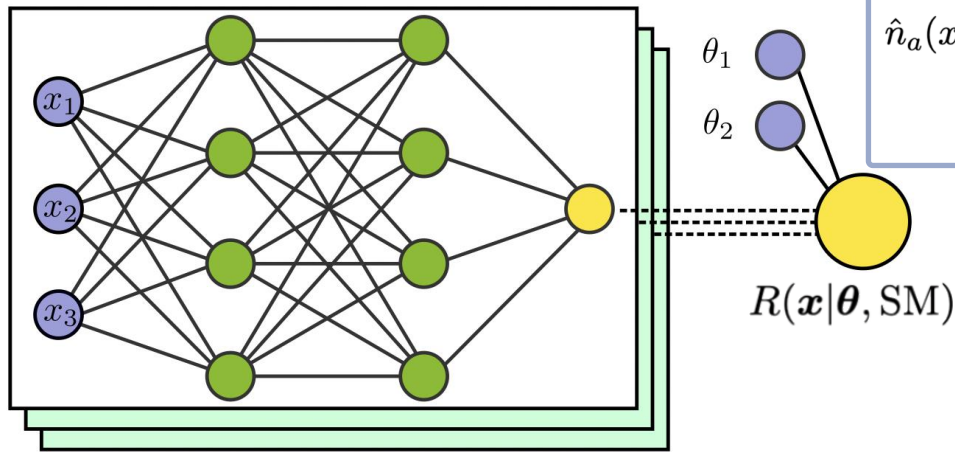
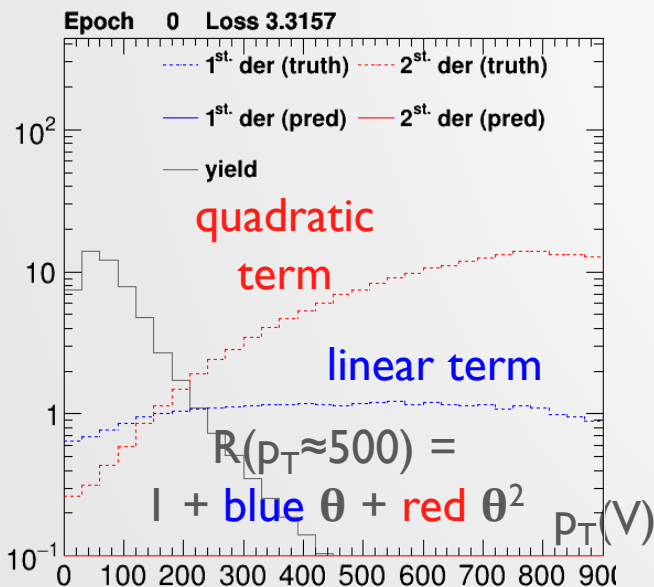
Similar to
 S. Chen, A. Glioti,
 G. Panico, A. Wulzer
[JHEP 05 \(2021\) 247](#)
[arXiv:2308.05704](#)

$$\hat{f}(x; \theta) = \frac{1}{1 + \hat{R}(x; \theta)}$$

invert likelihood trick

insert model knowledge:
 fit universal
 coefficient functions

$$\hat{R}(x; \theta) = \left(1 + \sum_a \theta_a \hat{n}_a(x) \right)^2 + \sum_a \left(\sum_{b \geq a} \theta_b \hat{n}_{ab}(x) \right)^2$$



$$\hat{n}_a(x) \rightarrow \frac{\partial_a p(x | \theta)}{p(x | \text{SM})} \Big|_{\theta = \text{SM}} = \frac{\partial_a \int dz p(x, z | \theta)}{\int dz p(x, z | \text{SM})} \Big|_{\theta = \text{SM}}$$

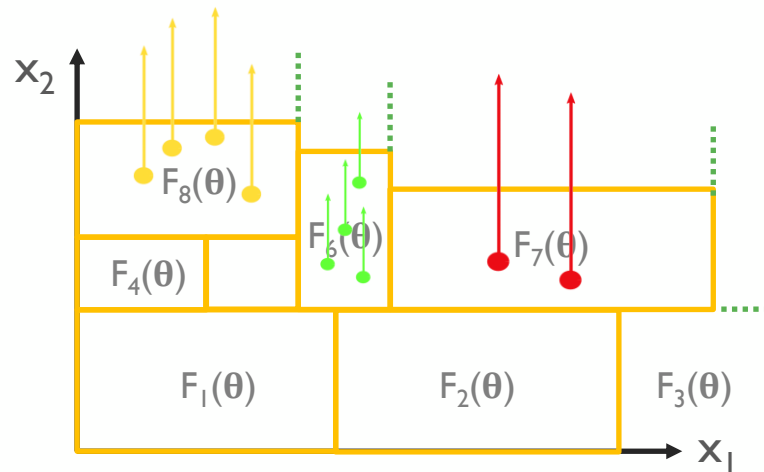
Integrates latent space!

Why would you
 want to use trees instead?

A SIMPLE TREE ALGORITHM

[[arXiv:2107.10859](https://arxiv.org/abs/2107.10859), [arXiv:2205.12976](https://arxiv.org/abs/2205.12976)]

phase-space partitioning



A simple tree

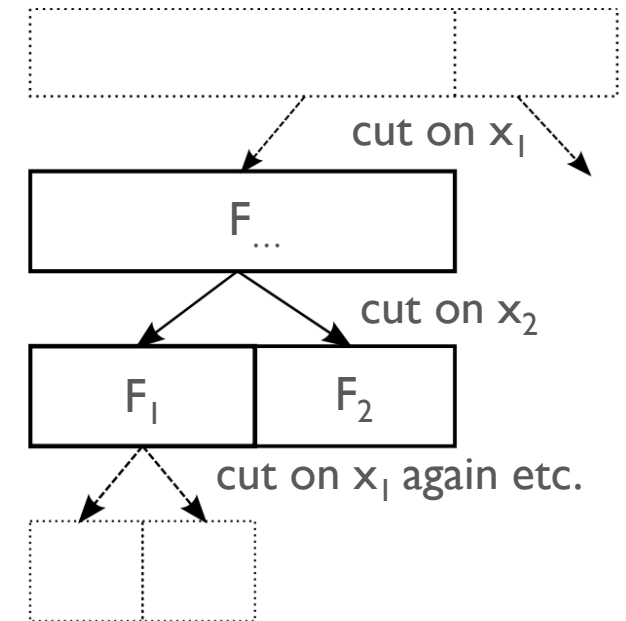
index-function (non-linearity)

$$\hat{F}(\mathbf{x}, \boldsymbol{\theta}) = \sum_{j \in \mathcal{J}} \mathbb{1}_j(\mathbf{x}) F_j(\boldsymbol{\theta})$$

phase space partitioning \mathcal{J} prediction F_j

need to solve for partitioning \mathcal{J} and $\{F_j\}$

training phase:
e.g. "CART" algo



- A tree is a hierarchical phase-space partitioning (\mathcal{J})
 - the novelty in the Boosted Information Tree is that we associate each region j with a polynomial $F_j(\boldsymbol{\theta})$
 - Note: A tree algorithm can have an arbitrarily complicated predictive function; here it is a SMEFT polynomial
- Fitting tree: Optimize "node split positions" on some loss. Trained (e.g. greedily) on the *ensemble*.

PARAMETRIC TREES FOR SMEFT

[[arXiv:2107.10859](https://arxiv.org/abs/2107.10859), [arXiv:2205.12976](https://arxiv.org/abs/2205.12976)]

Want to regress in r , exploiting its the polynomial θ dependence

$$r(x, z|\theta) = \frac{d\sigma(\mathbf{x}, \theta)/d\mathbf{x}}{d\sigma(\mathbf{x}, \text{SM})/d\mathbf{x}}$$

→ will allow to compute the optimal LLR test statistic $q(\mathcal{D})$

$$L = \sum_{\theta \in \mathcal{B}} \int d\mathbf{x} dz p(\mathbf{x}, z|\text{SM}) \left(r(x, z|\theta) - \hat{F}(\mathbf{x}, \theta) \right)^2$$

Tree ansatz

$F_j(\theta)$ polynomial with const. coeff.
(per node)

$$\hat{F}(\mathbf{x}, \theta) = \sum_{j \in \mathcal{J}} \underbrace{\mathbb{1}_j(\mathbf{x})}_{\text{find optimal partitioning}} \underbrace{F_j(\theta)}_{\text{find optimal predictor}}$$

Remove DOF from predictor:

$$F_j(\theta) = \frac{\sum_{i \in j} w_i(\theta)}{\sum_{i \in j} w_i(\theta_0)} \quad \text{sum up event weights within node \& divide}$$

No trainable parameters in the predictor
(Regression by means of classification)

Solve for optimal partitioning with greedy CART algorithm

$$L = - \sum_{\theta \in \mathcal{B}} \sum_{j \in \mathcal{J}} \frac{w_j^2(\theta)}{w_j(\theta_0)} = - \sum_{j \in \mathcal{J}} \sum_{\theta \in \mathcal{B}} \theta^a \theta^b I_{ab}^{(j)} + \mathcal{O}(\theta - \theta_0)^3$$

We're optimizing the Fisher information!

We'll find an optimized tree.
→ boost

CONCRETE SOLUTION: TREE BOOSTING

[arXiv:2107.10859, arXiv:2205.12976]

- Boosting: Fit model iteratively to pseudo-residuals of the preceding iteration with learning rate η

- Ansatz :
$$\hat{F}^{(b)}(\mathbf{x}, \boldsymbol{\theta}) = \underbrace{\hat{f}(\mathbf{x}, \boldsymbol{\theta})}_{\text{current iteration}} + \eta \underbrace{\hat{F}^{(b-1)}(\mathbf{x}, \boldsymbol{\theta})}_{\text{previous iteration}}$$

- Insert into the loss function:

$$L[\hat{f}^{(b)}] = \sum_{\boldsymbol{\theta} \in \mathcal{B}} \int d\mathbf{x} dz p(\mathbf{x}, z | \text{SM}) \left(r(\mathbf{x}, z | \boldsymbol{\theta}) - \underbrace{\eta \hat{F}^{(b-1)}(\mathbf{x}, \boldsymbol{\theta})}_{\text{previous iteration}} - \underbrace{\hat{f}^{(b)}(\mathbf{x}, \boldsymbol{\theta})}_{\text{current iteration}} \right)^2$$

current iteration

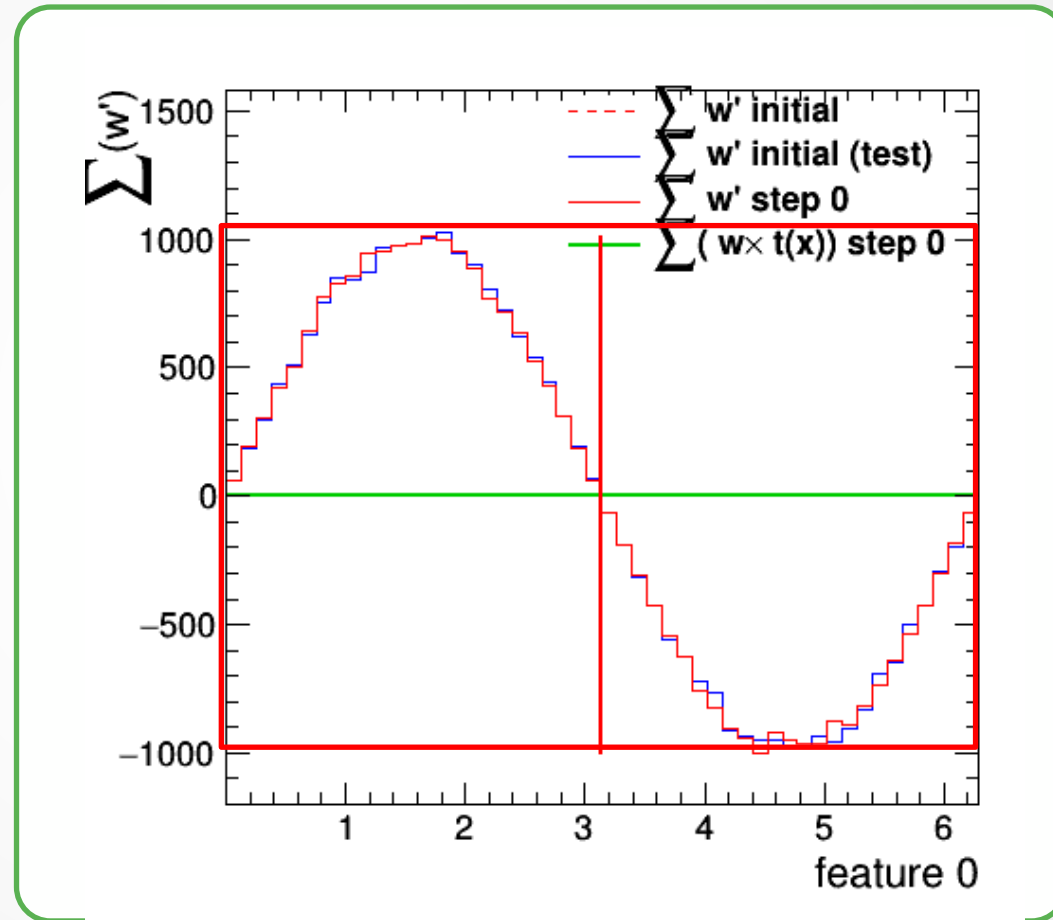
pseudo-residual, amounting to event-level reweighting

$$w_i^{(b)}(\boldsymbol{\theta}) \rightarrow w_i^{(b-1)}(\boldsymbol{\theta}) - \eta w_i^{(b-1)}(\boldsymbol{\theta}_0) \hat{F}^{(b-1)}(\mathbf{x}_i, \boldsymbol{\theta})$$

.... perform this iteratively
"Boosted Information Tree"

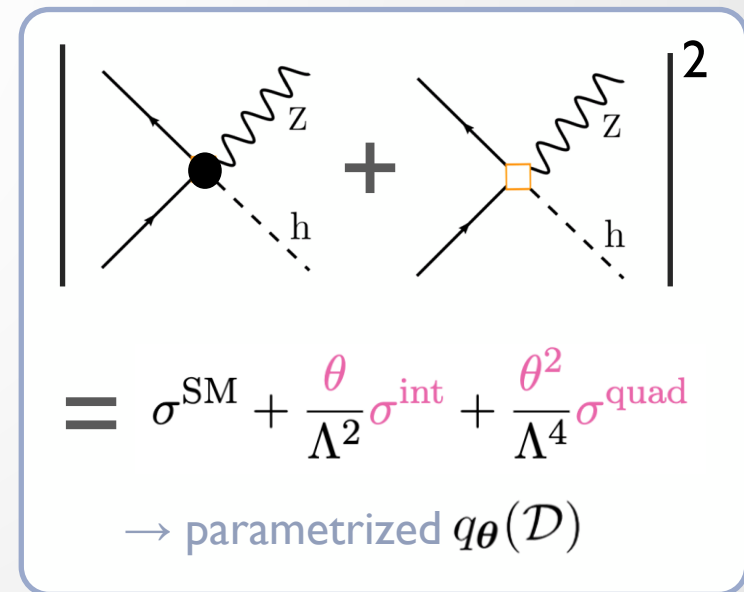
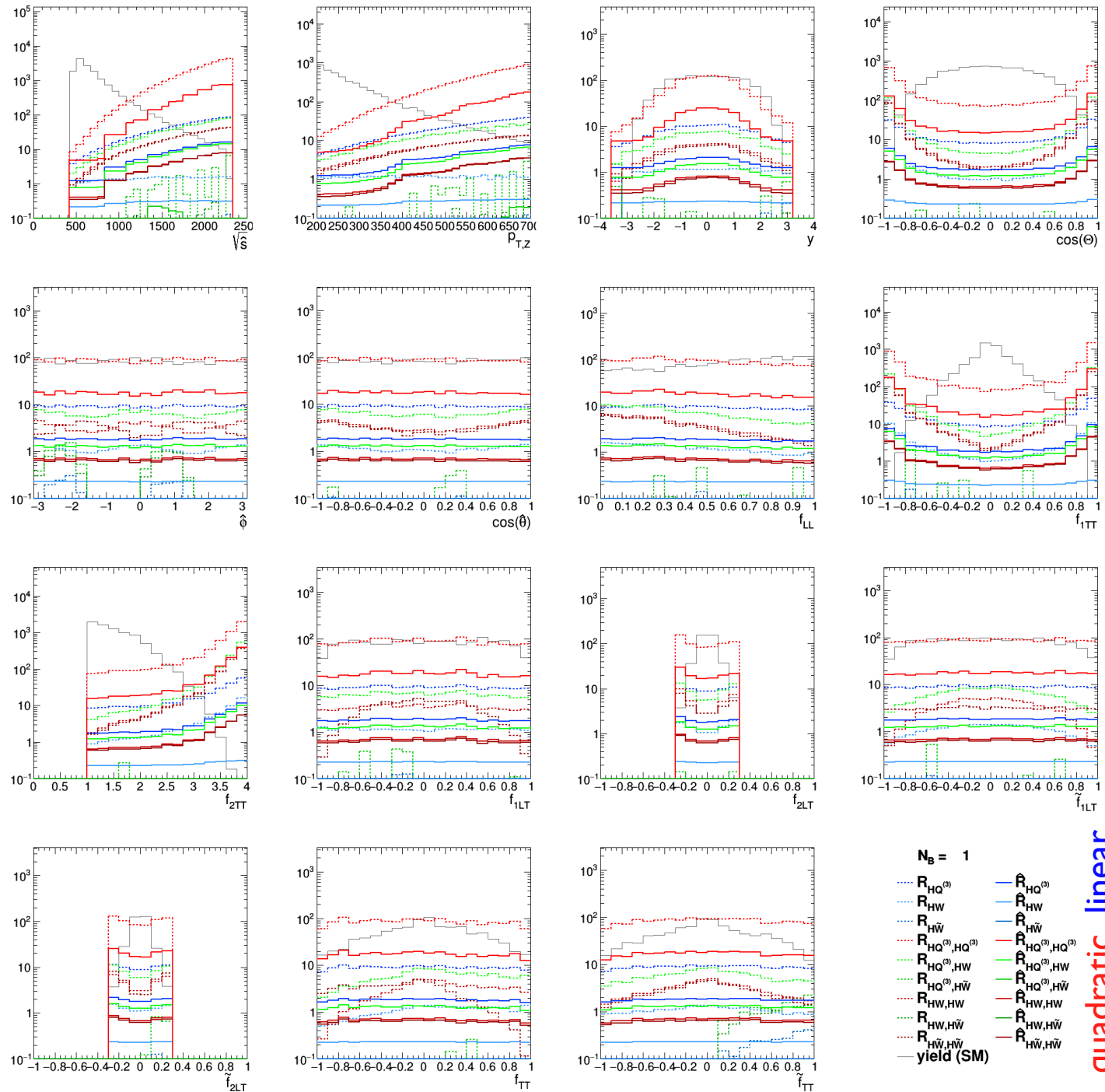
1D TOY EXAMPLE

- $\text{pdf}(x|\theta) = 1/(2\pi) - \theta \sin(x)$
- We predict the first derivative of the pdf wrt. to the parameter



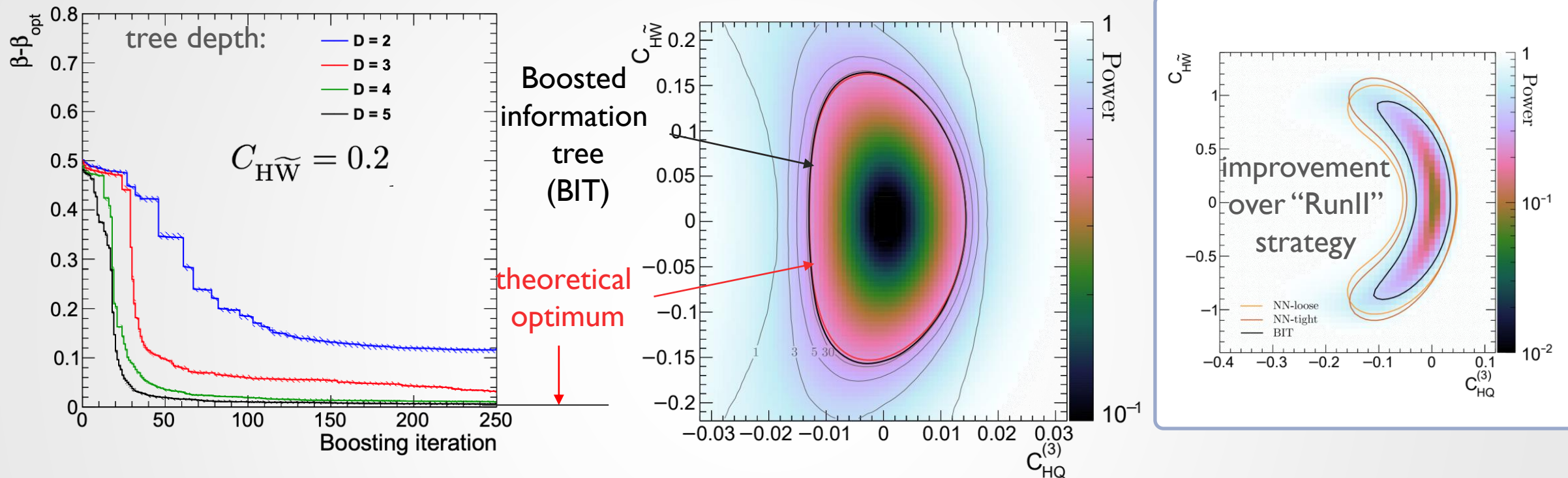
GIF animation not showing in pdf

- Realistic case: model of the ZH process
- “Boosted Information Tree (BIT)”
 - 3 WC, 9 DOF, 500k events, ZH
 - 200 trees, D=5, 9 minutes of training
 - also more realistic study, including backgrounds [[2107.10859](#)], [[2205.12976](#)]
- Learning coefficient functions to compute parametrized optimal observables



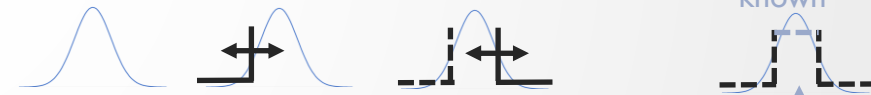
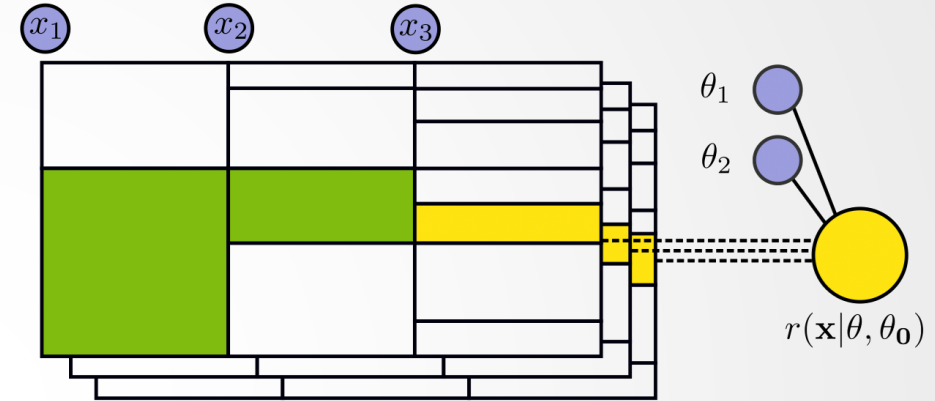
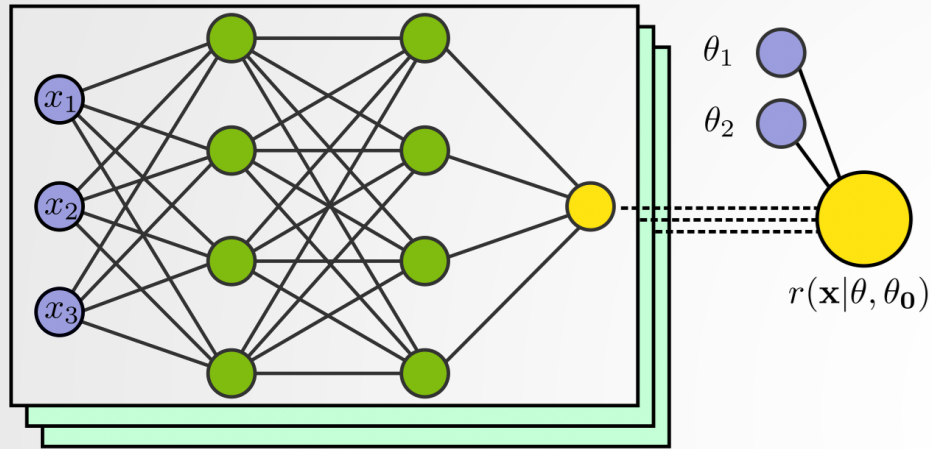
OPTIMALITY IN TEST CASES

[arXiv:2107.10859, arXiv:2205.12976]



- Obtain parametrized classifiers with 20-40% improvements in 2D toy cases (NOT marginalized!)
- No free lunch – Analysis dependent choices are needed
 - Binned analysis: variable binning \rightarrow background estimation is CPU intensive
 - Systematics treatment for unbinned analyses (beyond Higgs $M_{4\ell}$) less far developed
- Is it all worth it in higher dimensions? Yes! More examples: [[ML₄EFT](#)]; full list of references in backup

NETWORKS VS. TREES – WHAT IS THE BIG DEAL?



- Given a phase space region with EFT dependence: NN must select & predict
- In the Boosted Information Tree, the weak learner only selects
 - The prediction (F_j) is computed from the boxed events → **integrates latent space**
 - The regression problem is solved with **computational complexity** of classification
 - Speed advantage at high operator dimensions!

$$F_j(\boldsymbol{\theta}) = \frac{\sum_{i \in j} w_i(\boldsymbol{\theta})}{\sum_{i \in j} w_i(\boldsymbol{\theta}_0)} = \frac{\int dz \frac{d\sigma_{\boldsymbol{\theta}}}{d(x,z)}}{\int dz \frac{d\sigma_{SM}}{d(x,z)}}$$

SUMMARY!

- Various algorithms predict SMEFT dependence, mostly capitalizing on weighted simulation
 - Provide NP-optimal observables for hypothesis tests
- Trees **eliminate** the **latent space integration** and suitable to weight-based SMEFT predictions
- Parametrized classifiers “ask” for **unbinned analysis**

[[SWAN project](#)]

*Get in touch with
us for an in-person
walkthrough*

```
from MultiBoostedInformationTree import MultiBoostedInformationTree
bit = MultiBoostedInformationTree(
    training_features = training_features,
    training_weights = training_weights,
    base_points = base_points,
    feature_names = model.feature_names,
    **model.multi_bit_cfg
)
bit.boost()
test_predictions = bit.vectorized_predict(test_features)
```

+ 500 lines for figs

GOALS FOR MACHINE-LEARNING *OF* EFT

[EPJC 81 (2021) 178]

SMEFT effects can be

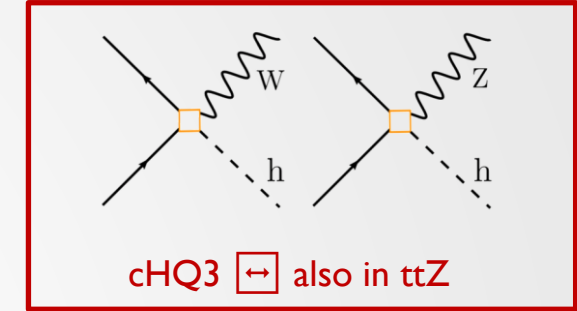
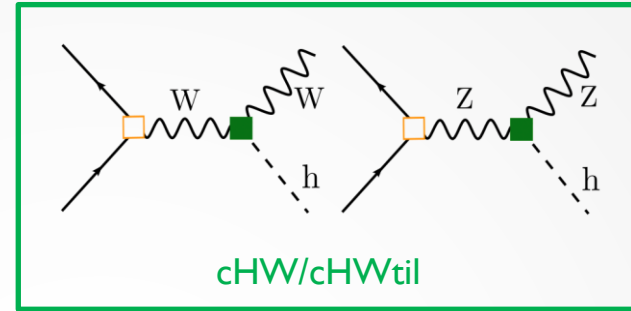
1. in the tails of the distributions because, e.g. 4-point functions grow with energy

2. in angular observables & correlations, sometimes encoding CP-violating effects

- “interference resurrection” [PLB 2017 11 086](#)
- “method of moments” [JHEP 06 \(2021\) 031](#)
- Enhance / single out the linear term
 - Up to triple-angular correlations, x5-10 boost in sensitivity

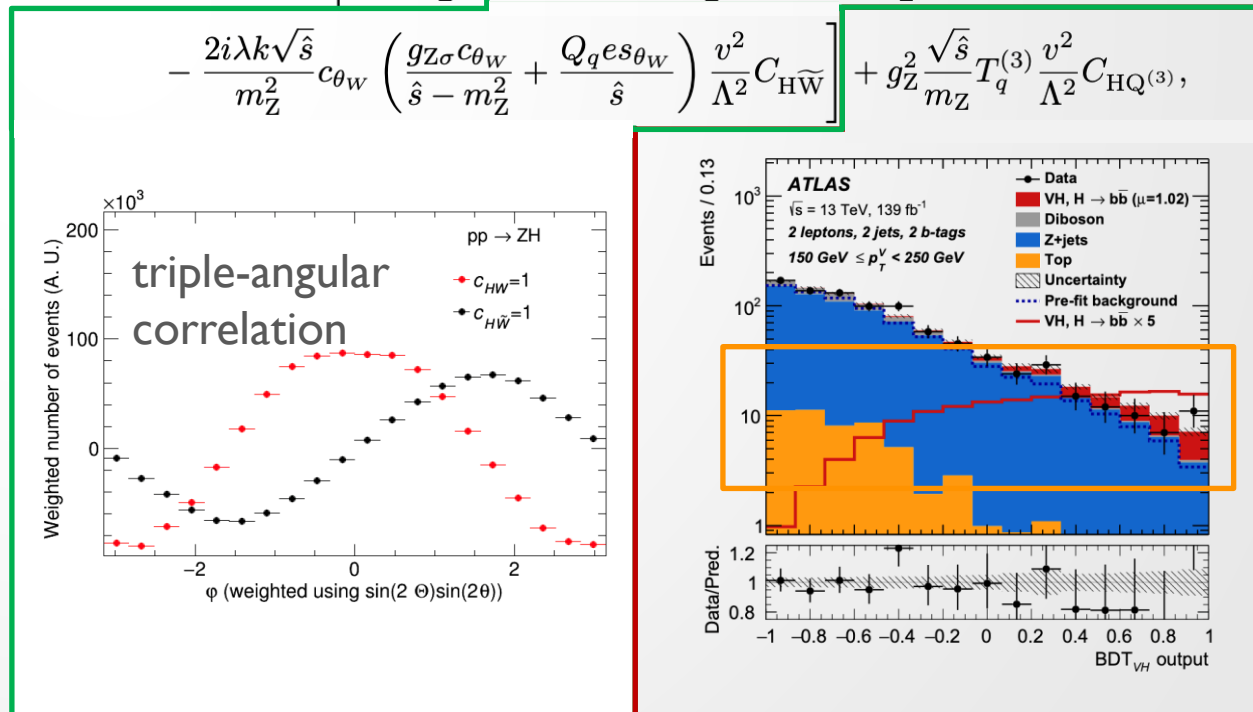
3. on top of “kinematically complex” backgrounds

- Def: Usually amenable to classification MVAs
- Unify the training target with classification



Tree-level SMEFT amplitude of ZH (transverse polarisation):

$$\hat{M}_\sigma^{\lambda=\pm} = g_Z m_Z \sqrt{\hat{s}} \left[\frac{g_{Z\sigma}}{\hat{s} - m_Z^2} + c_{\theta_W} \left(1 + \frac{\hat{s} - m_h^2}{m_Z^2} \right) \left(\frac{g_{Z\sigma} c_{\theta_W}}{\hat{s} - m_Z^2} + \frac{Q_q e s_{\theta_W}}{\hat{s}} \right) \frac{v^2}{\Lambda^2} C_{HW} - \frac{2i\lambda k \sqrt{\hat{s}}}{m_Z^2} c_{\theta_W} \left(\frac{g_{Z\sigma} c_{\theta_W}}{\hat{s} - m_Z^2} + \frac{Q_q e s_{\theta_W}}{\hat{s}} \right) \frac{v^2}{\Lambda^2} C_{H\tilde{W}} \right] + g_Z^2 \frac{\sqrt{\hat{s}}}{m_Z} T_q^{(3)} \frac{v^2}{\Lambda^2} C_{HQ^{(3)}}$$



HOW TO PARAMETRIZE?

- Quantum field theory: Differential cross section predict polynomial SM-EFT dependence:

$$d\sigma(\boldsymbol{\theta}) \propto |\mathcal{M}_{\text{SM}}(\mathbf{z}) + \boldsymbol{\theta}_a \mathcal{M}_{\text{BSM}}^a(\mathbf{z})|^2 d\mathbf{z} \quad \text{probability = wave function, squared}$$

- additivity of the matrix element \rightarrow incur a simple (polynomial) dependence in $\boldsymbol{\theta}$ for fixed configuration \mathbf{z}

$$\frac{d\sigma(\mathbf{x}, \boldsymbol{\theta})}{d\mathbf{x}} = \frac{d\sigma_{\text{SM}}(\mathbf{x})}{d\mathbf{x}} + \sum_a \theta_a \frac{d\sigma_{\text{int.}}^a(\mathbf{x})}{d\mathbf{x}} + \frac{1}{2} \sum_{a,b} \theta_a \theta_b \frac{d\sigma_{\text{BSM}}^{ab}(\mathbf{x})}{d\mathbf{x}}$$

- Neyman-Pearson: $q(\mathcal{D}) = \frac{L(\mathcal{D}|\boldsymbol{\theta})}{L(\mathcal{D}|\text{SM})}$ where $L(\mathcal{D}|\boldsymbol{\theta}) = \text{P}_{\mathcal{L}\sigma(\boldsymbol{\theta})}(N) \times \prod_{i=1}^N p(\mathbf{x}_i|\boldsymbol{\theta})$

“normalization” N “shape”

$$q_{\boldsymbol{\theta}}(\mathcal{D}) = \underbrace{\mathcal{L}(\sigma_{\boldsymbol{\theta}} - \sigma_{\text{SM}})}_{\text{const.}} - \sum_{\mathbf{x}_i \in \mathcal{D}} \log R(\mathbf{x}_i|\boldsymbol{\theta}, \text{SM})$$

Optimality can be achieved with cross-section ratio R or its universal coefficient functions R_a, R_{ab}

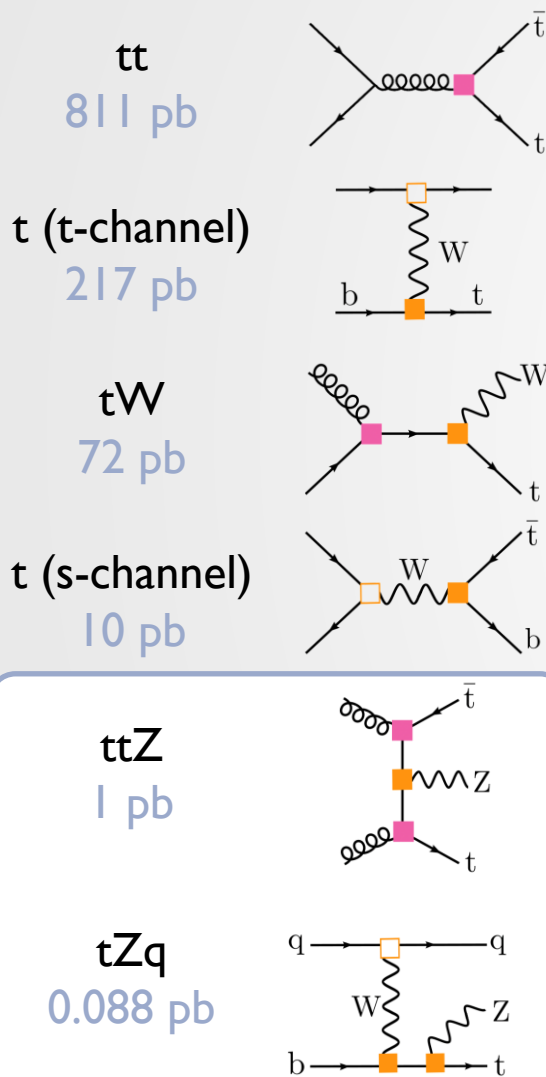
$$R(\mathbf{x}|\boldsymbol{\theta}, \text{SM}) = \frac{d\sigma(\mathbf{x}, \boldsymbol{\theta})/d\mathbf{x}}{d\sigma(\mathbf{x}, \text{SM})/d\mathbf{x}} = 1 + \sum_a \theta_a R_a(\mathbf{x}) + \frac{1}{2} \sum_{a,b} \theta_a \theta_b R_{ab}(\mathbf{x})$$

NB #1 Curse of dimensionality is lifted!!
15 operators \rightarrow 136 coefficients

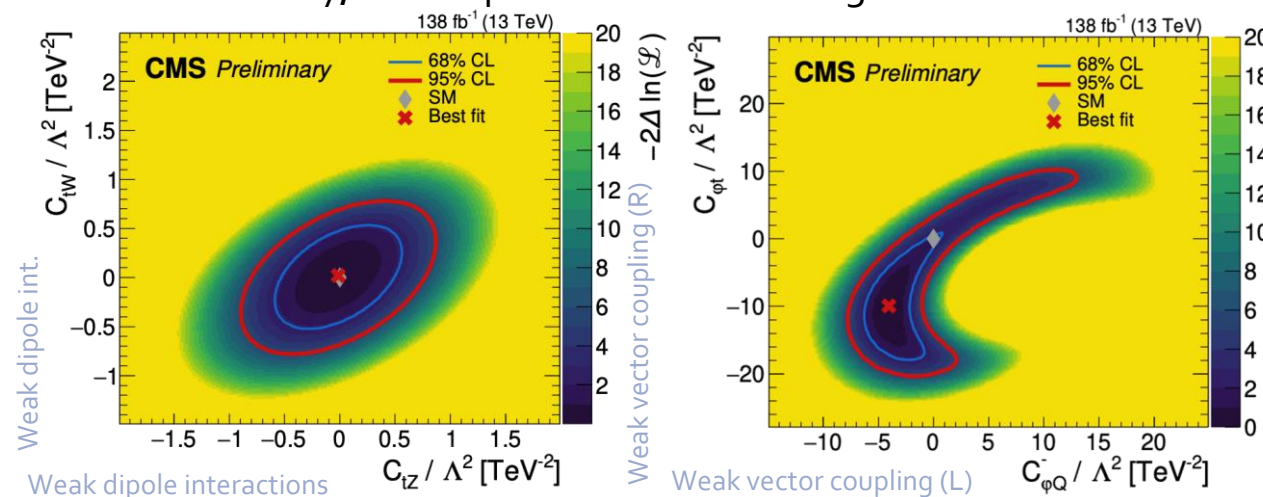
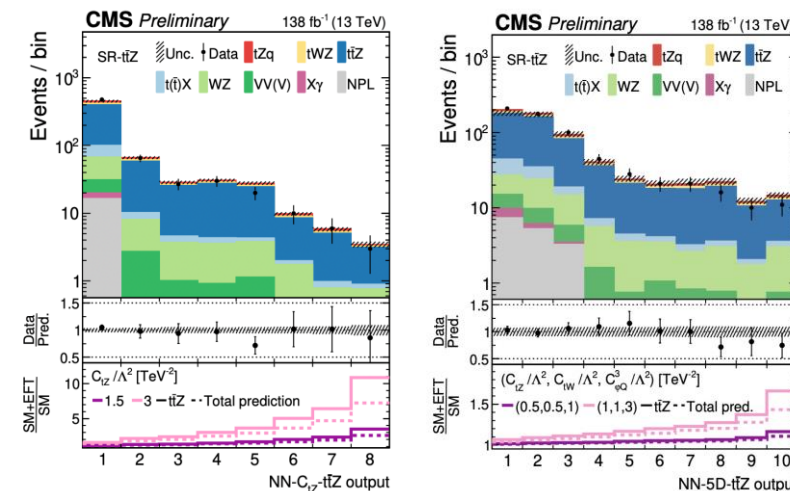
NB #2: R is positive: Fit universal dependence using the most general quadratic polynomial

$$\cong \left(1 + \sum_a \theta_a \hat{n}_a(\mathbf{x})\right)^2 + \sum_a \left(\sum_{b \geq a} \theta_b \hat{n}_{ab}(\mathbf{x})\right)^2$$

TOP QUARK PAIR + Z BOSON

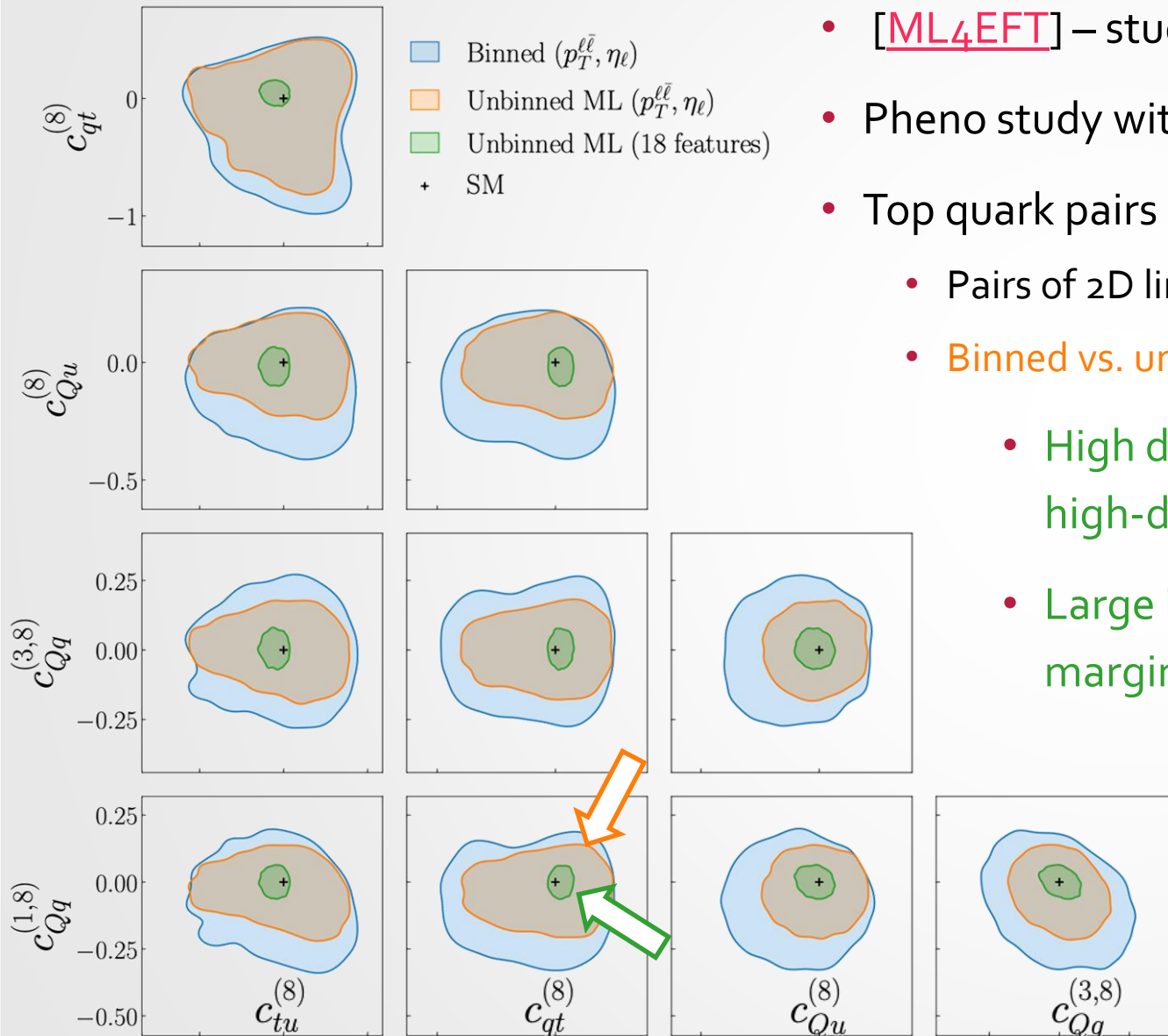


- Measure the top quark – Z boson coupling
- Train separate “SM vs. EFT” classifiers
 - Single operator O_{tZ} , O_{tW} , $O^3_{\phi Q}$
 - different trainings for different limits (!)
 - “likelihood trick” for SMEFT effects
- signal extraction with 1D, 2D, and 5D LL fit
 - Sampling of parameter space in the training
 - Targeted signals differ kinematically, but no parametrized training is used
 - Signal mix
 - no large linear terms \rightarrow OK
- Best current limits





IMPROVING HIGH DIMENSIONAL LIMITS

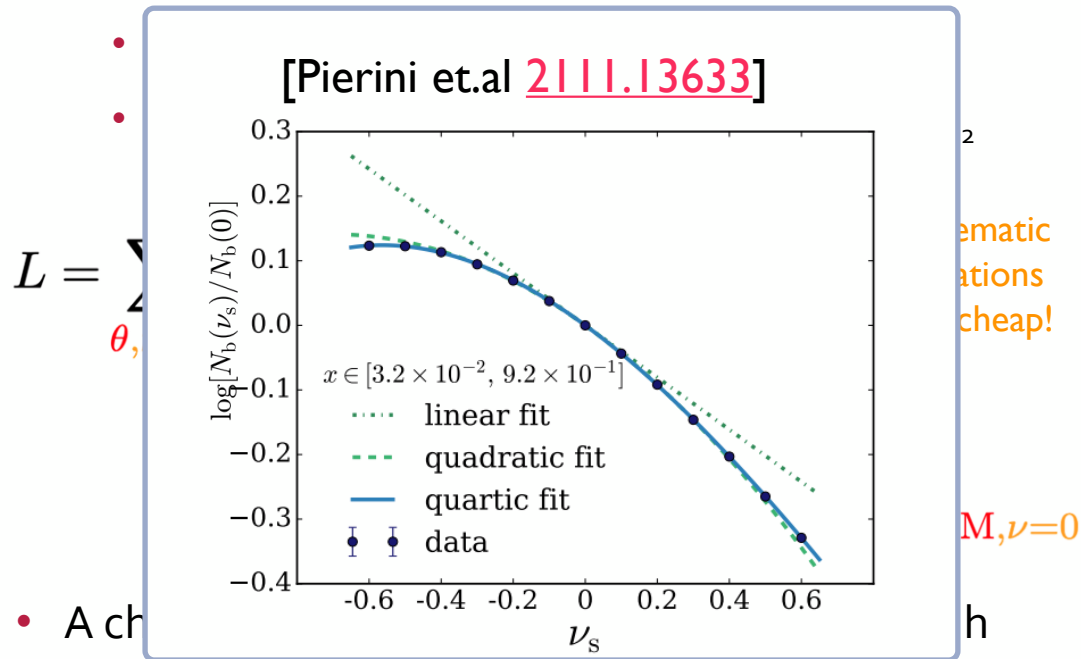


- [ML₄EFT] – study ZH and top quark pairs
- Pheno study with parametrized NN classifiers
- Top quark pairs in low ($N_f=2$) and high feature dimension $N_f=18$
 - Pairs of 2D limits with 6 more ops marginalized
 - Binned vs. unbinned: Some gain w/ unbinned when using 2 features
 - High dimensional observation ($N_f=18$) constraining a high-dimensional ($N_{\text{coef}}=8$) model using an SM candle
 - Large improvement for $N_f=18$ – mostly in the marginalized limits
- Take seriously constraining power from SM candle
- Whether the sensitivity gain survives systematics in an unbinned detector-level analysis is an open question

TOWARDS UNBINNED ANALYSIS

- Binned parametrized classifiers are impractical for high SMEFT parameter dimension

- What's missing to go all-in? Systematics.



- A change in event counts in the profiling
- Divide & conquer #1: Experiments begun machine-learning certain nuisances: h_{damp} , b-fragmentation

- Divide & conquer #2: Unbinned unfolding for high dimensions

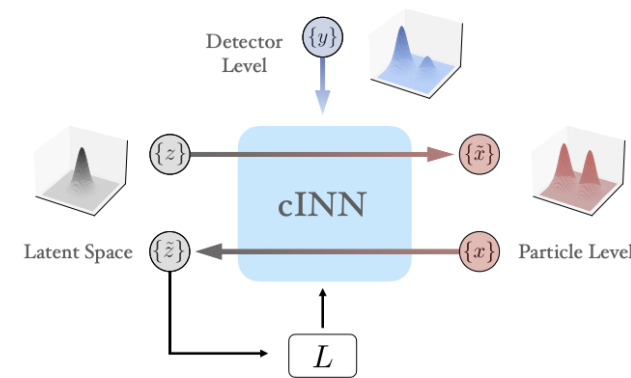
- Consider on the conditional pdf $p(x_{\text{det}} | z_{\text{ptl}})$ which can be evaluated in the forward mode

- Unfolding algorithms use Bayes' theorem

$$p(x_{\text{det}} | z_{\text{ptl}}) p(z_{\text{ptl}}) = p(z_{\text{ptl}} | x_{\text{det}}) p(x_{\text{det}})$$

- to learn $p(z_{\text{ptl}} | x_{\text{det}})$; GAN & other generative versions

- Mostly iterative, to remove simulated prior

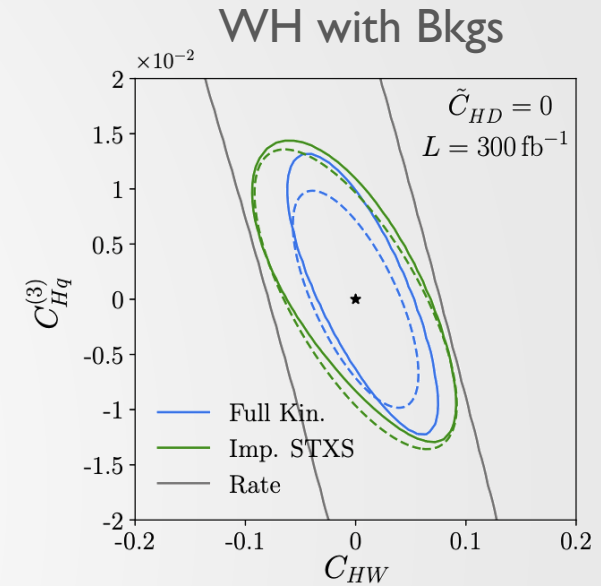


[community paper]
e.g. [OmniFold]
[cINN], [all]

- Report unbinned unfolded data; then SMEFT analysis

REFERENCES

- **Madminer**: Neural networks based likelihood-free inference & related techniques
 - K. Cranmer, J. Pavez, and G. Louppe [1506.02169]
 - J. Brehmer, K. Cranmer, G. Louppe, J. Pavez [1805.00013] [1805.00020] [1805.12244]
 - J. Brehmer, F. Kling, I. Espejo, K. Cranmer [1907.10621]
 - J. Brehmer, S. Dawson, S. Homiller, F. Kling, T. Plehn [1908.06980]
 - A. Butter, T. Plehn, N. Soybelman, J. Brehmer [2109.10414]
 - established many of the *main ideas* & *statistical interpretation* in various *NN applications*
- **Weight derivative regression** (A.Valassi) [2003.12853]
- **Parametrized classifiers** for SM-EFT: NN with quadratic structure
- S. Chen, A. Glioti, G. Panico, A. Wulzer [JHEP 05 (2021) 247] [arXiv:2308.05704]
- **Boosted Information Trees**: Tree algorithms & boosting
 - S. Chatterjee, S. Rohshap, N. Frohner, R.S., D. Schwarz [2107.10859], [2205.12976]
- **ML₄EFT** R. Ambrosio, J. Hoeve, M. Madigan, J. Rojo, V. Sanz [2211.02058]
- All approaches are “SMEFT-specific ML” with differences mostly on the practical side



my practical
experience

→ talk later today