

#### EXPLORING EFT WITH ML AT THE LHC

R. Schöfbeck (HEPHY Vienna), Sept. 8<sup>th</sup>, 2022



#### ACTIVITIES @ HEPHY (CMS DATA ANALYSIS)



#### How well is the Standard Model? – Inclusive cross sections

[all summary plots CMS and ATLAS]



#### **ATLAS SUSY Searches\* - 95% CL Lower Limits**

ATLAS SUSY Searches* - 95% CL Lower Limits March 2022							[all summary plots <u>CMS</u> and <u>ATLAS</u> ]			<b>ATLAS</b> Preliminary $\sqrt{s} = 13$ TeV		
	Model	S	ignature	e j	∫ <i>L dt</i> [fb <sup>−</sup>	']	Mass limit					Reference
Inclusive Searches	$ ilde{q} ilde{q},   ilde{q}  ightarrow q  ilde{\chi}_1^0$ $ ilde{q}  ilde{q},   ilde{q}  ightarrow q  ilde{\chi}_1^0$	0 <i>e</i> ,μ mono-jet 0 <i>e</i> ,μ	2-6 jets 1-3 jets 2-6 jets	$E_T^{\text{miss}}$ $E_T^{\text{miss}}$ $E_T^{\text{miss}}$	139 139 139	<ul> <li> <i>q</i> [1×, 8× Degen.]         <i>q</i>         [8× Degen.]         [9         [         [</li></ul>		1.0 0.9	1	2.3	$m(\tilde{\chi}_{1}^{0}) < 400 \text{ GeV}$ $m(\tilde{q}) - m(\tilde{\chi}_{1}^{0}) = 5 \text{ GeV}$ $m(\tilde{\chi}_{1}^{0}) = 0 \text{ GeV}$	2010.14293 2102.10874 2010.14293
	$\begin{split} \tilde{g}\tilde{g}, \ \tilde{g} \to q\bar{q}W\tilde{\chi}_{1}^{0} \\ \tilde{g}\tilde{g}, \ \tilde{g} \to q\bar{q}(\ell\ell)\tilde{\chi}_{1}^{0} \\ \tilde{g}\tilde{g}, \ \tilde{g} \to q\bar{q}WZ\tilde{\chi}_{1}^{0} \end{split}$	1 e,μ ee,μμ 0 e,μ SS e,μ	2-6 jets 2 jets 7-11 jets 6 jets	$E_T^{\text{miss}}$ $E_T^{\text{miss}}$	139 139 139 139	יבי יבי ובי ובי יבי איני		Forbidden	1.15	-1.95 2.2 2.2 1.97	$\begin{array}{c} m(\tilde{\chi}_{1}^{0}) \! = \! 1000 \; \mathrm{GeV} \\ m(\tilde{\chi}_{1}^{0}) \! < \! 600 \; \mathrm{GeV} \\ m(\tilde{\chi}_{1}^{0}) \! < \! 700 \; \mathrm{GeV} \\ m(\tilde{\chi}_{1}^{0}) \! < \! 600 \; \mathrm{GeV} \\ m(\tilde{g}) \! - \! m(\tilde{\chi}_{1}^{0}) \! = \! 200 \; \mathrm{GeV} \end{array}$	2010.14293 2101.01629 CERN-EP-2022-014 2008.06032 1909.08457
	$\tilde{g}\tilde{g},  \tilde{g} \rightarrow t t \tilde{\chi}_1^0$	0-1 <i>e</i> ,μ SS <i>e</i> ,μ	3 <i>b</i> 6 jets	$E_T^{\rm miss}$	79.8 139	ĩb B			1.25	2.25	$\mathfrak{m}(\widetilde{\chi}_1^0) < 200 \text{ GeV}$ $\mathfrak{m}(\widetilde{g}) \cdot \mathfrak{m}(\widetilde{\chi}_1^0) = 300 \text{ GeV}$	ATLAS-CONF-2018-041 1909.08457
3 <sup>rd</sup> gen. squarks direct production	$ ilde{b}_1 ilde{b}_1$	0 <i>e</i> , <i>µ</i>	2 b	$E_T^{\rm miss}$	139	$egin{array}{c}  ilde{b}_1 \  ilde{b}_1 \end{array}$		0.68	1.255	10	$m(\widetilde{\chi}_1^0){<}400GeV$ $\mathrm{O}GeV{<}\Deltam(\widetilde{b}_1,\widetilde{\chi}_1^0){<}20GeV$	2101.12527 2101.12527
	$\tilde{b}_1 \tilde{b}_1, \tilde{b}_1 \rightarrow b \tilde{\chi}_2^0 \rightarrow b h \tilde{\chi}_1^0$	0 <i>e</i> ,μ 2 τ	6 <i>b</i> 2 <i>b</i>	$E_T^{\mathrm{miss}}$ $E_T^{\mathrm{miss}}$	139 139	<i>b</i> <sub>1</sub> Forbidden <i>b</i> <sub>1</sub>		0.13-0.85	0.23-1.35	$\Delta m( ilde{\chi}^0_2, ilde{\chi}^0_1)=\ \Delta m( ilde{\chi}^0_2, ilde{\chi})$	= 130 GeV, m( $\tilde{\chi}_1^0$ )=100 GeV $\tilde{\chi}_1^0$ =130 GeV, m( $\tilde{\chi}_1^0$ )=0 GeV	1908.03122 2103.08189
	$ \begin{split} \tilde{t}_{1}\tilde{t}_{1}, \tilde{t}_{1} \rightarrow t\tilde{\chi}_{1}^{0} \\ \tilde{t}_{1}\tilde{t}_{1}, \tilde{t}_{1} \rightarrow Wb\tilde{\chi}_{1}^{0} \\ \tilde{t}_{1}\tilde{t}_{1}, \tilde{t}_{1} \rightarrow \tilde{t}_{1}bv, \tilde{\tau}_{1} \rightarrow \tau\tilde{G} \\ \tilde{t}_{1}\tilde{t}_{1}, \tilde{t}_{1} \rightarrow c\tilde{\chi}_{1}^{0} / \tilde{c}\tilde{c}, \tilde{c} \rightarrow c\tilde{\chi}_{1}^{0} \end{split} $	0-1 e, μ 1 e, μ 1-2 τ 0 e, μ 0 e, μ	$\geq$ 1 jet 3 jets/1 b 2 jets/1 b 2 c mono-jet	$E_T^{\text{miss}} \\ E_T^{\text{miss}} \\ E_T^{\text{miss}} \\ E_T^{\text{miss}} \\ E_T^{\text{miss}}$	139 139 139 36.1 139	<ul> <li> <i>˜</i><sub>1</sub> <i>˜</i><sub>1</sub> <i>˜</i><sub>1</sub> <i>˜ ˜</i></li></ul>	Forbidde	n 0.65 Forbidden 0.85	1.25		$\begin{split} m(\tilde{\chi}_{1}^{0}) = &1 \ {\rm GeV} \\ m(\tilde{\chi}_{1}^{0}) = &500 \ {\rm GeV} \\ m(\tilde{\tau}_{1}) = &800 \ {\rm GeV} \\ m(\tilde{\tau}_{1}^{0}) = &0 \ {\rm GeV} \\ m(\tilde{\tau}_{1}, \tilde{c}) - m(\tilde{\chi}_{1}^{0}) = &5 \ {\rm GeV} \end{split}$	2004.14060,2012.03799 2012.03799 2108.07665 1805.01649 2102.10874
	$\tilde{t}_1\tilde{t}_1, \tilde{t}_1 \rightarrow \tilde{\mathcal{K}}_2^0, \tilde{\mathcal{X}}_2^0 \rightarrow Z/h\tilde{\mathcal{X}}_1^0$ $\tilde{t}_2\tilde{t}_2, \tilde{t}_2 \rightarrow \tilde{t}_1 + Z$	1-2 e,μ 3 e,μ	1-4 <i>b</i> 1 <i>b</i>	$E_T^{ m miss} \ E_T^{ m miss}$	139 139	$ ilde{t}_1 \\  ilde{t}_2$	Forbidder	0.067 0.86	-1.18	$m(\tilde{\chi}_1^0)=360$	$m(\widetilde{\chi}_2^0){=}500~{ m GeV}$ GeV, $m(\widetilde{t}_1){-}m(\widetilde{\chi}_1^0){=}40~{ m GeV}$	2006.05880 2006.05880
Long-lived particles	Direct $\tilde{\chi}_1^* \tilde{\chi}_1^-$ prod., long-lived $\tilde{\chi}_1^\pm$	Disapp. trk	1 jet	$E_T^{\rm miss}$	139	$ \tilde{\chi}_{1}^{\pm} \\ \tilde{\chi}_{1}^{\pm} $ 0.21		0.66			Pure Wino Pure higgsino	2201.02472 2201.02472
	Stable $\tilde{g}$ R-hadron Metastable $\tilde{g}$ R-hadron, $\tilde{g} \rightarrow qq \tilde{\chi}_1^0$ $\tilde{\ell}\tilde{\ell}, \ \tilde{\ell} \rightarrow \ell \tilde{G}$	pixel dE/dx pixel dE/dx Displ. lep		$E_T^{\text{miss}}$ $E_T^{\text{miss}}$ $E_T^{\text{miss}}$	139 139 139 139	$\begin{array}{ccc} \tilde{g} \\ \tilde{g} & [\tau(\tilde{g}) = 10 \text{ ns}] \\ \tilde{e}, \tilde{\mu} \\ \tilde{\tau} \\ \tilde{\tau} \end{array}$	0.34	0.7		2.05 2.2	$\mathfrak{m}(\widetilde{\chi}_1^0)$ =100 GeV $ au(\widetilde{\ell})$ = 0.1 ns	CERN-EP-2022-029 CERN-EP-2022-029 2011.07812
RPV	$\begin{split} \tilde{\chi}_{1}^{\pm} \tilde{\chi}_{1}^{\mp} / \tilde{\chi}_{1}^{0} , \tilde{\chi}_{1}^{\pm} \rightarrow \mathbb{Z}\ell \rightarrow \ell\ell\ell \\ \tilde{\chi}_{1}^{\pm} \tilde{\chi}_{1}^{\mp} / \tilde{\chi}_{2}^{0} \rightarrow WW/\mathbb{Z}\ell\ell\ell\ell\nu\nu \\ \tilde{g}\tilde{g} , \tilde{g} \rightarrow qq\tilde{\chi}_{1}^{0} , \tilde{\chi}_{1}^{0} \rightarrow qqq \end{split}$	3 <i>e</i> ,μ 4 <i>e</i> ,μ	0 jets 4-5 large jets	$E_T$ $E_T^{miss}$	139 139 36.1	$ \begin{split} \tilde{\chi}_{1}^{*} / \tilde{\chi}_{1}^{0} & [\text{BR}(Z\tau) = 1, \text{BR}(Ze) \\ \tilde{\chi}_{1}^{\pm} / \tilde{\chi}_{2}^{0} & [\lambda_{i33} \neq 0, \lambda_{12k} \neq 0] \\ \tilde{g} & [m(\tilde{\chi}_{1}^{0}) = 200 \text{ GeV}, 1100 \text{ GeV} \end{split} $	=1] GeV]	<ul> <li>no tell-tale signals in model-dependent searches</li> <li>push mass scale into the multi-TeV regime; here: SUSY</li> </ul>				
	$\begin{split} &\tilde{t}\tilde{t}, \tilde{t} \rightarrow t\tilde{\chi}_{1}^{0}, \tilde{\chi}_{1}^{0} \rightarrow tbs \\ &\tilde{t}\tilde{t}, \tilde{t} \rightarrow b\tilde{\chi}_{1}^{\pm}, \tilde{\chi}_{1}^{\pm} \rightarrow bbs \\ &\tilde{t}_{1}\tilde{t}_{1}, \tilde{t}_{1} \rightarrow bs \\ &\tilde{t}_{1}\tilde{t}_{1}, \tilde{t}_{1} \rightarrow d\ell \end{split}$	2 <i>e</i> ,μ 1 μ	Multiple $\geq 4b$ 2 jets + 2 b 2 b DV		36.1 139 36.7 36.1 136	$\begin{array}{c} \tilde{i}  [\lambda''_{323} = 2e \cdot 4, 1e \cdot 2] \\ \tilde{i} \\ \tilde{i}_1 \\ \tilde{i}_1  [qq, bs] \\ \tilde{i}_1 \\ \tilde{i}_1  [1e \cdot 10 < \lambda'_{334} < 1e \cdot 8, 3e \cdot 1] \\ \end{array}$	<i>Fort</i> <b>0.42</b> -10< λ' <3e-9]	• Are we	doing it	right?		
	$\tilde{\chi}_1^{\pm}/\tilde{\chi}_2^0/\tilde{\chi}_1^0, \tilde{\chi}_{1,2}^0 \rightarrow tbs, \tilde{\chi}_1^+ \rightarrow bbs$	1-2 e, µ	≥6 jets		139	$\tilde{\chi}_1^0$	0.2-0.32	• mo	odel inde	ependent?	$\rightarrow$ ``anomaly	detection"
*Only pher	Duly a selection of the available mass limits on new states or 10 <sup>-1</sup>						<ul> <li>search deviations compatible with SM symmetries         → "effective" theories</li> </ul>					

## WHERE TO LOOK AT THE LHC?

- Let's add all terms compatible with the SM symmetries
  - respect SM symmetries: SU(3)<sub>c</sub> ⊗ SU(2)<sub>L</sub>⊗U(1)
  - 59 operators at d=6 [JHEP10(2010)085]



• SM-EFT effects are polynomial modifications with varying coefficients over feature space

 $\left( \varphi^{\dagger} \varphi - \frac{v^2}{2} \right) W_{I}^{\mu 
u} W_{\mu 
u}^{I}$  ${\cal O}_{arphi W}$ 

coupling modifications or new interactions

## CONFRONT THE MODEL WITH COLLIDER DATA



## THE LIKELIHOOD FUNCTION

arxiv:1503.0x7622



#### DISENTANGLING SM-EFT IN THE HIGGS-SECTOR











- example #1: ZZ\* decay channel in all production modes
- experimentally clean ("golden channel")
- 10 = 5 (+5 CP odd) operators:  $c_{HW}$ ,  $c_{HB}$ ,  $c_{HW}$ ,  $c_{UH}$ ,  $c_{HWB}$
- attempt to optimally disentangle production modes



Reconstructed bins contain a mixture of production channels and backgrounds (mostly ZZ\*)



- ML is used to separate production modes in each category
- per reco-channel: NNs trained with 2-7 observables
  - combine with RNNs (LSTMs) using variable-length jets and leptons
  - common network layer for multiclassification in e.g., ggF, VBF, ZZ\*











## TTH IN THE MULTILEPTON CHANNEL







• example #2: t(t)H multilepton in 2 $\ell$ SS+o $\tau$ , 2 $\ell$ SS+1 $\tau$ , 3 $\ell$  final states

JHEP (submitted)

- 3 DNNs for signal/background multi-classification
- targets t-t-H Yukawa coupling (**=**) in *κ*-framework

• in SM-EFT: "CP" structure (complex phase) of  $HH^\dagger ar{q}_P u_r ilde{H}$ 

- use ML for separating CP-even vs. odd effects
  - gradient-BDT <u>XGBoost</u>
  - 38 input features (kinematic properties)



## TTH IN THE MULTILEPTON CHANNEL





- BDT exploits the likelihood trick to obtain CP even/odd fraction from the data
- limits on deviations of the t-t-H interaction (  $\kappa_{\rm t}$  ,  $\widetilde{\kappa}_{\rm t}$ ) including combinations with other final states
- example of learning "of" SM-EFT effects
- issue: large top backgrounds from ttZ and ttW in all measurement regions → combine sectors!
- $\tau$  lepton ID performance has significant impact

# **INTERLUDE: CLASSIFICATION WITH DEEPTAU**

real  $\tau_{\rm h}$ 

seven  $\tau$  decay

modes

[INST 17 (2022) P07023 sketch from Izaak Neuteligns

μ



- 5 hadronic + 2 leptonic decays •
- three main fake contributions
- new [DeepTau] identification algorithm classifies  $\tau_{\rm h}$  modes
- similar to
  - ATLAS *τ* ID [<u>using RNNs</u>]
  - [DeepJet] for g/c/b/uds/leptons • identification and
  - [DeepAK8] for t/W/Z/H decays ٠
- high level candidate-features (fully connected) and feature *maps* on two grids of all particles in the vicinity in convolutional layers
- 140M  $\tau$  candidates, 690hrs ٠



charged tracks

+ ECAL clusters



# INTERLUDE: CLASSIFICATION WITH DEEPTAU

- $\tau$  leptons in the detector
  - 5 hadronic + 2 leptonic decays
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Applied similarly for inner and outer cells



INTERLUDE: CLASSIFICATION WITH DEEPTAU

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improvement of background suppression by almost factor 2 when compared to previous  $\tau$  MVA not using the convolutional layers





#### **RECENT SM-EFT RESULTS (SELECTION!)**



#### **RECENT SM-EFT RESULTS (SELECTION!)**



#### **TOP AND DIBOSON SECTORS**



## SM-EFT EFFECTS ARE EVERYWHERE





- Solve background correlations like a triangular matrix (i.e. staged):
  - Multi-differential high-dimensional SM-EFT analysis of candles:
    - Drell-Yan, W+Jets, ttbar, single-top (t), etc.
  - Then move to ZH (+ Drell-Yan), WH (+ttbar),  $H \rightarrow WW$  (+WW and ttbar)
- Can go in parallel provided re-interpretation is feasible
  - Needs close-to complete likelihood → a whole separate discussion
- ML versatile tools to optimally extract SM-EFT effects without too much tuning need → parametrized classifiers are an example





## EXPLOITING PARAMETRIZED SIMULATION WITH TREE ALGOS



• Quantum field theory: Differential cross section have structure

 $\mathrm{d}\sigma(\boldsymbol{\theta}) \propto |\mathcal{M}_{\mathrm{SM}}(\boldsymbol{z}) + \boldsymbol{\theta}_a \mathcal{M}_{\mathrm{BSM}}^a(\boldsymbol{z})|^2 \mathrm{d}\boldsymbol{z}$ 

- sampling z at a fixed θ<sub>o</sub>
- re-evaluate the likelihood for a few alternative  $\boldsymbol{\theta}$
- fix polynomial coefficients of event weights w<sub>i</sub>(θ)

$$w_i(\boldsymbol{\theta}) = w_{i,0} + \sum_a w_{i,a} \,\theta_a + \frac{1}{2} \sum_{a,b} w_{ab} \,\theta_a \theta_b = \frac{\sigma(\boldsymbol{\theta})}{\sigma(\boldsymbol{\theta}_0)} \cdot r(\boldsymbol{x}_i, \boldsymbol{z}_i | \boldsymbol{\theta}, \boldsymbol{\theta}_0)$$

SM interference SM-EFT

interpretation valid at LO

probability =

wave function,

squared

• obtain predictions *parametrized* in  $\theta$ 

from MC simulation run in "forward mode"

## **TREES & BOOSTING**



- Let us make a tree-based ansatz for the differential cross-section ratio R
- The "weak learner" is a tree associating a sub-region (j) of a partitioning  $\mathcal J$  with a predictive function  $F_i$
- Fitting tree: Optimize "node split positions" on some loss. Trained (e.g. greedily) on the *ensemble*.
  - An axis-aligned tree is limited. Remove the limitation iteratively with "boosting".

## LEARNING MORE WITH TREES



## **CONCRETE SOLUTION: TREE BOOSTING**

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

• Ansatz : 
$$\hat{F}^{(b)}(\boldsymbol{x},\boldsymbol{\theta}) = \hat{f}(\boldsymbol{x},\boldsymbol{\theta}) + \eta \hat{F}^{(b-1)}(\boldsymbol{x},\boldsymbol{\theta})$$

currentpreviousiterationiteration

• Insert into the loss function:

.... perform this iteratively



#### [arXiv:2107.10859, arXiv:2205:12976]

- "Boosted Information tree" (BIT)
- 500 k events, 3 WCs, 9 coefficients
  - 9 minutes training
- Tested in a ZH toy model, and a more realistic Delphes study, including backgrounds



## OPTIMALITY IN TOY DATA

- Test with toy simulation in ZH final state unbinned likelihood ratio test statistic
- Neyman-Pearson: The LL ratio test statistic has the highest power (1-β) for a given test size (CL=95%)



- tree depth D=4 sufficient. Instead of the unbinned case, N<sub>bin</sub> = 5 already very close to optimum
- significant improvement when including backgrounds and comparing to conventional Run-II strategy

## THE SM-EFT CHALLENGE IS NOT ABOUT ML

- Methods to parametrize (close-to) optimal observables for the various final states are established
- The challenge is a 100+ combination (aka global fit) that we can trust
  - across all processes,
  - across all operators,
  - across many years of experimental developments,
  - and while theoretical predictions improve
- The important groundwork is on what we publish, and how complete (uncertainties & correlations), and reproducible it is.
  - ML algorithms help to semi-automatize the analysis design while we can stay receptive to new theory ideas





#### NEURAL NETWORKS REGRESS; THE BIT DOESN'T



- Each NN layer maps  $L_{n+1} = \sigma(W_{ij} L_n + b_i)$ . These DOF need to select & predict the regressed values.
- In the BIT, we only select. The prediction (F<sub>j</sub>) is computed from the boxed events. This is possible, because a tree algorithm is (greedely) trained on the *ensemble*. The BITs' DOF are NOT updated event-by-event.

## WW AND H $\rightarrow$ WW\* COMBINATION (LEPTONIC)

- Preformed combined fit of
  - **1**. signal strengths of ggH and VBF in  $H \rightarrow WW^*$
  - 2. SM WW unfolded differential p<sub>T</sub>(lead-.l) x-sec
- 20 SM-EFT operators affecting the measurements
- physics-guided eigenbasis probes 8 directions
  - Assume a U(3)<sup>5</sup> flavor symmetry
- Stepping stone for more global EFT combinations
- STXS combination: [ATLAS-CONF-2020-053]





ATL-PHYS-PUB-2021-010, 36fb<sup>-1</sup>

### WW AND $H \rightarrow WW^*$ COMBINATION

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## LIKELIHOOD RATIO TRICK

arxiv:1503.0x7622

Neyman-Pearson Lemma: The likelihood **ratio** 

$$q(\mathcal{D}) = rac{L(\mathcal{D}|oldsymbol{ heta})}{L(\mathcal{D}|oldsymbol{ heta}_0)} \sim \sum_{i=1}^N \log rac{p(oldsymbol{x}_i|oldsymbol{ heta})}{p(oldsymbol{x}_i|oldsymbol{ heta}_0)}$$

is the optimal test- statstic in hypothesis tests



Provides the lowest mis-identification probability for a given signal efficieny (No free parameters! ↔ simple hypothesis) • Train a discriminator to separate signal from background and regress in the truth label

$$L = \int d\mathbf{x} \sum_{z \in \{0,1\}} p(\mathbf{x}, z) \left(z - \hat{f}(\mathbf{x})\right)^2$$
training sample
with mixture of
signal (1) and bkg (0)
$$= \int d\mathbf{x} \left( p(\mathbf{x}, 0) \hat{f}(\mathbf{x})^2 + p(\mathbf{x}, 1)(1 - \hat{f}(\mathbf{x}))^2 \right)$$

• Training, e.g., with p(z=o) = p(z=1)

$$f^*(x) = rac{p(x,1)}{p(x,1) + p(x,0)} = rac{1}{1 + r(x)}$$

"Likelihood ratio trick" provides a close-to optimal test statistic

Let's look at SM-EFT applications & issues ... 34

## LHC LONG TERM SCHEDULE



~ factor 10 more data (~5 10<sup>34</sup> cm<sup>-2</sup>s<sup>-1</sup>) 3 ab<sup>-1</sup>

ng
r

Last updated: January 2022

## SENDING MIXED SIGNALS TO THE LOSS FUNCTION

$$L = \sum_{\theta \in \mathcal{B}} \int d\mathbf{x} \left( p(\mathbf{x}|\theta) \hat{f}(\mathbf{x})^2 + p(\mathbf{x}|SM)(1 - \hat{f}(\mathbf{x}))^2 \right)$$
  
mixing signals &  
case dependent mixes  
$$f^*(\mathbf{x}) = \frac{1}{1 + r_{\mathcal{B}}(\mathbf{x})} \qquad r_{\mathcal{B}}(\mathbf{x}) = \frac{\frac{1}{|\mathcal{B}|} \sum_{\theta \in \mathcal{B}} p(\mathbf{x}|\theta)}{p(\mathbf{x}|SM)}$$

- MSE (& cross-entropy) loss functions average the training data set
  - less-than-ideal for linear effects
- Does not reflect what we know about the heta dependence
- The real issue is the necessity for a case-dependent training
- The challenge of global SM-EFT searches will require a high degree of automatization
  - Need strategies for learning (approximations) of the log-likelihood suitable for high parameter dimensions

## HOW TO PARAMETRIZE?

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

 $\mathrm{d}\sigma(oldsymbol{ heta}) \propto |\mathcal{M}_{\mathrm{SM}}(oldsymbol{z}) + oldsymbol{ heta}_a \mathcal{M}^a_{\mathrm{BSM}}(oldsymbol{z})|^2 \mathrm{d}oldsymbol{z}$ 

probability = wave function, squared

• additivity of the matrix element  $\rightarrow$  incur a simple (polynomial) dependence in  $\theta$  for fixed configuration z

$$\frac{\mathrm{d}\sigma(\boldsymbol{x},\boldsymbol{\theta})}{\mathrm{d}\boldsymbol{x}} = \frac{\mathrm{d}\sigma_{\mathrm{SM}}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} + \sum_{a} \theta_{a} \frac{\mathrm{d}\sigma_{\mathrm{int.}}^{a}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} + \frac{1}{2} \sum_{a,b} \theta_{a} \theta_{b} \frac{\mathrm{d}\sigma_{\mathrm{BSM}}^{ab}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}}$$

• Neyman-Pearson: 
$$q(\mathcal{D}) = \frac{L(\mathcal{D}|\boldsymbol{\theta})}{L(\mathcal{D}|\mathrm{SM})}$$
 where  $L(\mathcal{D}|\boldsymbol{\theta}) = P_{\mathcal{L}\sigma(\boldsymbol{\theta})}(N) \times \prod_{i=1}^{N} p(\boldsymbol{x}_i|\boldsymbol{\theta})$   
 $q_{\boldsymbol{\theta}}(\mathcal{D}) = \mathcal{L}(\sigma_{\boldsymbol{\theta}} - \sigma_{\mathrm{SM}}) - \sum_{\boldsymbol{x}_i \in \mathcal{D}} \log R(\boldsymbol{x}_i|\boldsymbol{\theta}, \mathrm{SM})$  Optimality can be achieved with cross-section ratio R or its universal coefficient functions  $R_a$ ,  $R_{ab}$   
 $\mathcal{R}(\boldsymbol{x}|\boldsymbol{\theta}, \mathrm{SM}) = \frac{\mathrm{d}\sigma(\boldsymbol{x}, \boldsymbol{\theta})/\mathrm{d}\boldsymbol{x}}{\mathrm{d}\sigma(\boldsymbol{x}, \mathrm{SM})/\mathrm{d}\boldsymbol{x}} = 1 + \sum_{a} \theta_a R_a(\boldsymbol{x}) + \frac{1}{2} \sum_{a,b} \theta_a \theta_b R_{ab}(\boldsymbol{x})$   
NB #1 Curse of dimensionality is lifted!! NB #2: R is positive: Fit universal dependence using the most general quadratic polynomial  $\hat{\boldsymbol{x}} = \left(1 + \sum_{a} \theta_a \hat{n}_a(\boldsymbol{x})\right)^2 + \sum_{a} \left(\sum_{b \geq a} \theta_b \hat{n}_{ab}(\boldsymbol{x})\right)^2$ 

## OPTIMAL PARAMETRIZED CLASSIFIERS

• studied in the context of  $p \ p \to W^{\pm} \ Z \to (l^{\pm} \ \nu) \ (l^{+} \ l^{-})$  for the most important SM-EFT operators







JHEP 05 (2021) 247

JHEP 07 (2022) 032

ATLAS-CONF-NOTE-2016-043

- high purity, ~85%-90% as seen by <u>ATLAS</u> and <u>CMS</u> (with SM-EFT)
- Adam optimizer, pytorch, 10<sup>4</sup> epochs, learning rate of 10<sup>-4</sup>
  - 4 hidden layers á 32 nodes, 2 networks simultaneously trained
  - alternatives configurations studied
- establish optimality with analytic model (Toy), very similar at (N)LO

## **PYTORCH IMPLEMENTATION**

- ZH production, analytic model, 500k events
  - Single coefficient: c<sub>HW</sub> (tested with up to 3)
  - 4 hidden layers á 32 nodes, 2 networks simultaneously trained
  - 10<sup>4</sup> epochs, Adam optimizer, LR=10<sup>-4</sup>
- The training is *simultaneous* and it must be!
  - Positivity is a property of the polynomial, not of an individual coefficient.
- several options to emphasise the tails
  - bias loss with function of A(x) or choosing base points
- just a proof of principle implementation



K. Cranmer , J. Pavez , and G. Louppe J. Brehmer, K. Cranmer, G. Louppe, J. Pavez J. Brehmer, F. Kling, I. Espejo, K. Cranmer [<u>1506.02169]</u> [<u>1805.00013</u>] [<u>1805.00020</u>] [<u>1805.12244</u>] [<u>1907.10621</u>]

#### • It's somewhat of a miracle that one can regress on the observable-level likelihood ratio

Observables	Integration over intractable factors	Detector & reconstruction	Parton shower		Parton-level momenta	Theory parameters
$p(oldsymbol{x} oldsymbol{ heta}) =$	$\int \mathrm{d} oldsymbol{z}_{\mathrm{d}}  \mathrm{d} oldsymbol{z}_{\mathrm{s}}  \mathrm{d} oldsymbol{z}_{\mathrm{p}}  p(oldsymbol{x} oldsymbol{z})$	$oldsymbol{z}_{ m d}) \qquad p($	$oldsymbol{z}_{ m d} oldsymbol{z}_{ m s})$	$p(oldsymbol{z}_{\mathrm{s}} oldsymbol{z}_{\mathrm{p}})$	$p(oldsymbol{z}_{ ext{p}})$	$ m{ heta})$
$q_{o}(\mathcal{D}) = \text{const} -$	$\sum \log \frac{\sigma(\boldsymbol{\theta})}{2} \frac{p(\boldsymbol{x}_i   \boldsymbol{\theta} )}{2}$		$\mathrm{d}\sigma( heta$	$) \propto$		
$q_{\theta}(\mathcal{D}) = \text{const.}$	$\sum_{\boldsymbol{x}_i \in \mathcal{D}} \log \sigma(\boldsymbol{\theta}_0) p(\boldsymbol{x}_i   \boldsymbol{\theta}_0)$		$ \mathcal{M}_{ ext{SM}}(oldsymbol{z})+oldsymbol{ heta} $			${\cal M}^a_{ m BSM}(oldsymbol{z}) ^2 { m d}oldsymbol{z}$
					calcuable & r	e-calcuable
super	powers				(aka tractable) th	eory prediction

based on this talk: <u>C. Kranmer, J. Brehmer</u>

## "JOINT" DISTRIBUTIONS ARE MUCH SIMPLER

- To understand the power of simulation, look at the simpler "joint" pdf
- 1. The intractable factors cancel in the joint LR

$$r(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}, \boldsymbol{\theta}_{0}) \equiv \frac{p(\boldsymbol{x}, \boldsymbol{z}_{d}, \boldsymbol{z}_{s}, \boldsymbol{z}_{p} | \boldsymbol{\theta})}{p(\boldsymbol{x}, \boldsymbol{z}_{d}, \boldsymbol{z}_{s}, \boldsymbol{z}_{p} | \boldsymbol{\theta}_{0})} = \frac{p(\boldsymbol{x} | \boldsymbol{z}_{d})}{p(\boldsymbol{x} | \boldsymbol{z}_{d})} \frac{p(\boldsymbol{z}_{d} | \boldsymbol{z}_{s})}{p(\boldsymbol{z}_{d} | \boldsymbol{z}_{s})} \frac{p(\boldsymbol{z}_{s} | \boldsymbol{z}_{p})}{p(\boldsymbol{z}_{s} | \boldsymbol{z}_{p})} \frac{p(\boldsymbol{z}_{p} | \boldsymbol{\theta})}{p(\boldsymbol{z}_{p} | \boldsymbol{\theta}_{0})} \propto \frac{|\mathcal{M}(\boldsymbol{z}_{p} | \boldsymbol{\theta})|^{2}}{|\mathcal{M}(\boldsymbol{z}_{p} | \boldsymbol{\theta}_{0})|^{2}}$$
Change in likelihood of observation x (with history z) going from  $\boldsymbol{\theta}_{0}$  to  $\boldsymbol{\theta}$  Intractable factors cancel re-calcuable theory prediction

2. Now fit a general function on the join space with a regressor depending only on the observables:

$$L = \int d\boldsymbol{x} d\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_0) \left( f(\boldsymbol{x}, \boldsymbol{z}) - \hat{f}(\boldsymbol{x}) \right)^2 \longrightarrow \min \qquad f^*(\boldsymbol{x}) = \frac{\int d\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_0) f(\boldsymbol{x}, \boldsymbol{z})}{\int d\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_0)} \qquad L$$

Latent space is integrated

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3. Now chose  $f(x,z) = r(x,z | \theta, \theta_o)$  which is available in simulation & fit with expressive function:

$$f^{*}(\boldsymbol{x}) = \frac{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0}) f(\boldsymbol{x}, \boldsymbol{z})}{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})} = \frac{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0}) p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})}{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})} = \frac{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})}{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})} = \frac{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})}{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})} = \frac{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})}{\int \mathrm{d}\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_{0})} = \frac{p(\boldsymbol{x} | \boldsymbol{\theta})}{p(\boldsymbol{x} | \boldsymbol{\theta}_{0})} = \frac{p(\boldsymbol{x} | \boldsymbol{\theta})}{p(\boldsymbol{x} | \boldsymbol{\theta}_{0})}$$
Available from simulation

... statistical framework of all the parametrized classifiers

#### EXPLOITING PARAMETRIZED SIMULATION WITH TREES



 $\theta_{1}$ 

 $\mathrm{d}\sigma(\boldsymbol{\theta}) \propto |\mathcal{M}_{\mathrm{SM}}(\boldsymbol{z}) + \boldsymbol{\theta}_a \mathcal{M}^a_{\mathrm{BSM}}(\boldsymbol{z})|^2 \mathrm{d}\boldsymbol{z}$ 

- sampling z at a fixed θ<sub>o</sub>
- evaluate  $d\sigma(\theta)$  for sufficient number of base-points  $\theta$
- fix polynomial coefficients of event weights w<sub>i</sub>(θ)

$$w_{i}(\boldsymbol{\theta}) = w_{i,0} + \sum_{a} w_{i,a} \theta_{a} + \frac{1}{2} \sum_{a,b} w_{ab} \theta_{a} \theta_{b} = \frac{\sigma(\boldsymbol{\theta})}{\sigma(\boldsymbol{\theta}_{0})} \cdot r(\boldsymbol{x}_{i}, \boldsymbol{z}_{i} | \boldsymbol{\theta}, \boldsymbol{\theta}_{0})$$
SM interference pure interpretation valid at LO

• obtain predictions for, e.g., yields for all x,z and  $\theta$ 

probability =

wave function,

squared

#### EXPLOITING PARAMETRIZED SIMULATION WITH TREES



• Quantum field theory: Differential cross section have structure

 $\mathrm{d}\sigma(oldsymbol{ heta}) \propto |\mathcal{M}_{\mathrm{SM}}(oldsymbol{z}) + oldsymbol{ heta}_a \mathcal{M}^a_{\mathrm{BSM}}(oldsymbol{z})|^2 \mathrm{d}oldsymbol{z}$ 

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## **TREES & BOOSTING**



- Let us make a tree-based prediction for R or its coefficient function
- Weak learner: Tree  $\leftrightarrow$  Associates a predictive function  $F_i$  (flexible!) with a sub-region j of a partitioning
- Fitting tree: Optimize "node split positions" on some loss. Trained (e.g. greedily) on the ensemble.
  - Rectangular cuts are very limiting. Remove the limitation with "boosting".

• Example: Learn a local version of the model, described by the score function (local LLR)

$$oldsymbol{t}(oldsymbol{x}|oldsymbol{ heta}_0) = 
abla_{oldsymbol{ heta}} \log p(oldsymbol{x}|oldsymbol{ heta}) igg|_{oldsymbol{ heta}_0} = rac{
abla_{oldsymbol{ heta}} p(oldsymbol{x}|oldsymbol{ heta})}{p(oldsymbol{x}|oldsymbol{ heta})} igg|_{oldsymbol{ heta}_0}$$

• Only the joint score  $t(x, z | \theta_0)$  is available in training. This is enough, though.

$$L = \int d\boldsymbol{x} \, d\boldsymbol{z} \, p(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_0) \left( t_a(\boldsymbol{x}, \boldsymbol{z} | \boldsymbol{\theta}_0) - \hat{F}_a(\boldsymbol{x}) \right)^2 \longrightarrow \min \qquad \text{formal solution:} \quad F_a^*(\boldsymbol{x}) = t_a(\boldsymbol{x} | \boldsymbol{\theta}_0)$$
$$= \sum_{(\boldsymbol{x}, \boldsymbol{z}, w)_i \in \mathcal{D}} w_{i,0} \left| \frac{w_{i,a}}{w_{i,0}} - \hat{F}_a(\boldsymbol{x}_i) \right|^2 = \sum_{j \in \mathcal{J}} \sum_{i \in j} w_i \left| \frac{w_{i,a}}{w_i} - F_j \right|^2 = \sum_{i=1}^{N_{\text{sim}}} \frac{w_{i,a}^2}{w_i} - 2 \sum_{j \in \mathcal{J}} F_j \sum_{i \in j} w_{i,a} + \sum_{j \in \mathcal{J}} F_j^2 \sum_{i \in j} w_i$$

$$\begin{split} \frac{\partial L}{\partial F_j} &= 0 \quad \longrightarrow \quad F_j = \frac{\sum_{i \in j} w_{i,a}}{\sum_{i \in j} w_i} & \text{ ...re-insert } F_j \text{ into } L \dots \\ & \text{the predictor does NOT have trainable parameters!} \\ L &= -\sum_{j \in \mathcal{J}} \frac{\left(\sum_{i \in j} w_{i,a}\right)^2}{\sum_{i \in j} w_i} = -\sum_{j \in \mathcal{J}} I^{(\lambda_j)} \text{ maximise Fisher information of a Poisson } \theta_a \text{ measurement} \end{split}$$

## **CONCRETE SOLUTION: TREE BOOSTING**

• Boosting: Fit linear model iteratively to pseudo-residuals of the preceding iteration

• Ansatz : 
$$\hat{F}^{(b)}(\boldsymbol{x}) = \hat{f}^{(b)}(\boldsymbol{x}) + \eta \hat{F}^{(b-1)}(\boldsymbol{x})$$
  
• Insert into the loss function: current previous iteration



.... perform this iteratively

## LEARNING MORE WITH TREES

Regress in one of the coefficient functions of R  
$$R(x|\theta, SM) = \frac{d\sigma(x,\theta)/dx}{d\sigma(x, SM)/dx}$$
  
 $= 1 + \sum_{a} \theta_{a}R_{a}(x) + \frac{1}{2} \sum_{a,b} \theta_{a}\theta_{b}R_{ab}(x)$ Regress in R, including its the polynomial  $\theta$  dependence  
 $R(x|\theta, SM) = \frac{d\sigma(x,\theta)/dx}{d\sigma(x, SM)/dx}$  $L = \int dx dz p(x, z|SM) \left(R_{a(,b)}(x, z) - \hat{F}_{a(,b)}(x)\right)^{2}$   
Tree ansatz for each a, ab: $\hat{F}(x) = \sum_{j \in \mathcal{J}} \mathbb{1}_{j}(x)F_{j}$   
 $\sum_{i \in j} w_{i}$ Tree ansatz for each a, ab: $\hat{F}(x) = \sum_{j \in \mathcal{J}} \mathbb{1}_{j}(x)F_{j}$   
 $\sum_{i \in j} w_{i}$ ... Solve for F<sub>i</sub> & reinsert ... $F_{j} = \frac{\sum_{i \in j} w_{i,ab}}{\sum_{i \in j} w_{i}}$ Solve for optimal partitioning with CART algorithm  
 $L = -\sum_{j \in \mathcal{J}} \frac{\left(\sum_{i \in j} w_{i,ab}\right)^{2}}{\sum_{i \in j} w_{i}}$ Solve for optimal partitioning with CART algorithm  
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## TTH IN THE MULTILEPTON CHANNEL







- example #2: t(t)H multilepton in  $2\ell SS+o\tau$ ,  $2\ell SS+1\tau$ ,  $3\ell$  final states
- deep convolutional network [DeepTau] for  $\tau$  reconstruction
  - uses tracking, calorimetry, muons via particle-flow collections
- 3 DNNs for signal/background multi-classification
- targets t-t-H Yukawa coupling (**=**) in *κ*-framework
  - in SM-EFT: "CP" structure (complex phase) of  $~HH^\dagger {ar q}_P u_r ilde H$
  - CP violating effects in couplings to bosons ( $\blacksquare$ ) supressed by  $\Lambda^4$
- use ML for separating CP-even vs. odd: gradient-BDT <u>XGBoost</u>
  - 38 input features (kinematic properties)



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JHEP (submitted

### INCLUDING BACKGROUNDS IN THE TRAINING [arXiv:2107.10859, arXiv:2205:12976]



- Include most important background processes
  - Simulate signal using MG5 & SMEFTsim + Delphes
  - learn R(x|0) for ZH + Drell-Yan (correctly weighted)
- Train on observables that capture EFT dependence and also discriminate between backgrounds
- Compare with the CMS "Run II" strategy: NN to separate background, then fit  $p_T(Z)$ 
  - substantial improvement

## **TOP QUARKS + X IN SM-EFT**

tt

811 pb

217 pb

tW

72 pb

t (s-channel)

10 pb

ttΖ

l pb

tZq

0.088 pb

W

 $\sim Z$ 

2000



example #3: top quark – Z boson coupling 00000 exploit kinematics in ttZ/tZq/tWZ final states low-background final states; bkg for tt+Higgs t (t-channel) 5 SM-EFT operators  $\mathcal{S}^{W}$ Extensive use of MVAs 

- Multiclassifier to discriminate between several SM processes
  - using 33 (mostly kinematic) event properties
- 8 neural network binary classifiers to BSM events "NN-SM" tΖα  $\cap$ ()()Bkgs

 $\mathcal{O}_{tZ}$ Weak top dipole interactions  $\mathcal{O}_{\mathrm{tW}}$  $\mathcal{O}^3_{\varphi \mathrm{Q}}$ LH vector couplings  ${\cal O}^-_{\varphi {
m Q}}$ RH vector couplings  $\mathcal{O}_{\varphi \mathsf{t}}$ 

2 or 3 hidden layers 50-100 neurons **ReLU** activation. sigmoid output LR 0.001 (decaying) Adam optimizer



#### **TOP AND DIBOSON SECTORS**



	Decay mode	Resonance	B (%)
	Leptonic decays		35.2
	$ au^-  ightarrow { m e}^- \overline{ u}_{ m e}  u_{ au}$		17.8
	$ au^-  ightarrow \mu^- \overline{ u}_\mu  u_ au$		17.4
	Hadronic decays		64.8
charge-conjugate decays.	$ au^-  ightarrow { m h}^-  u_ au$		11.5
	$ au^-  ightarrow { m h}^- \pi^0  u_ au$	ho (770)	25.9
	$ au^-  ightarrow { m h}^- \pi^0 \pi^0  u_ au$	$a_1(1260)$	9.5
	$ au^-  ightarrow { m h}^- { m h}^+ { m h}^-  u_ au$	$a_1(1260)$	9.8
	$ au^-  ightarrow \mathrm{h}^-\mathrm{h}^+\mathrm{h}^-\pi^0  u_ au$		4.8
	Other		3.3