Machine Learning in Top Physics in the CMS Collaboration

Philip Keicher on behalf of the CMS Collaboration
New Brunswick, November 3rd, 2022

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

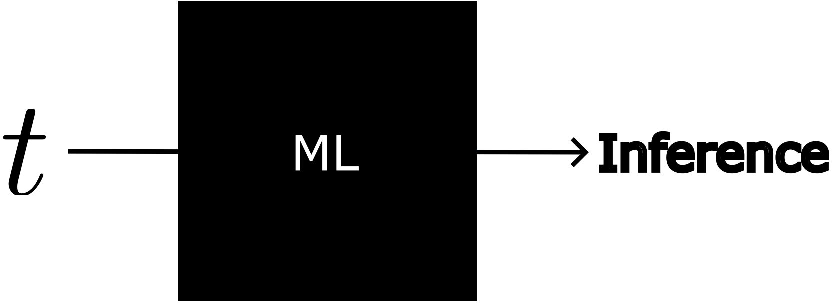
GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung

Special thanks to
Kai-Feng Chen, Valentina Guglielmi, Jan Kieseler and Melissa Quinnan
for providing material!

Introduction

$t \longrightarrow$ **Inference**

Introduction



- ML-techniques standard for many aspects of top-related physics

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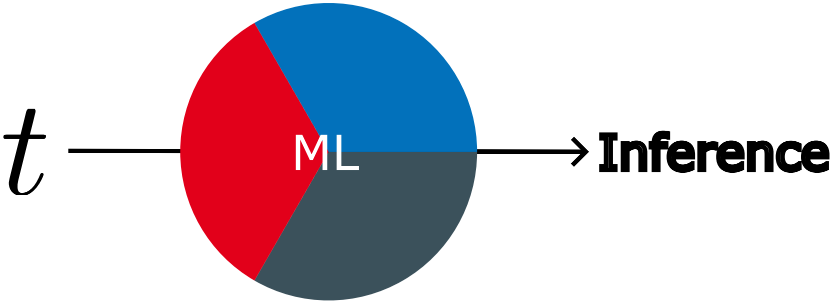

- ML-techniques standard for many aspects of top-related physics
  - Tagging [b-tagging (CMS)] [top-tagging landscape paper]
  - Reconstruction
  - Construction of final observable

$\rightarrow$ Multitude of different strategies and architectures

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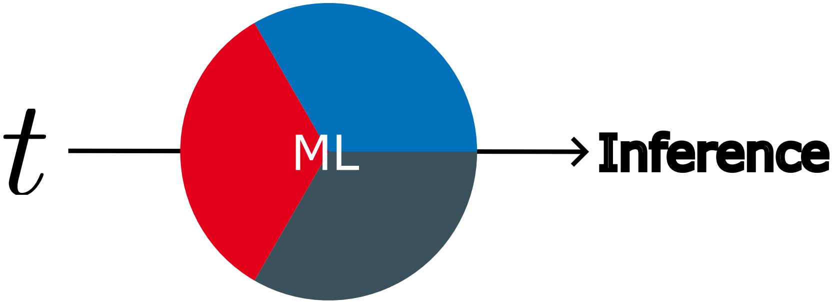

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$\rightarrow$ Multitude of different strategies and architectures

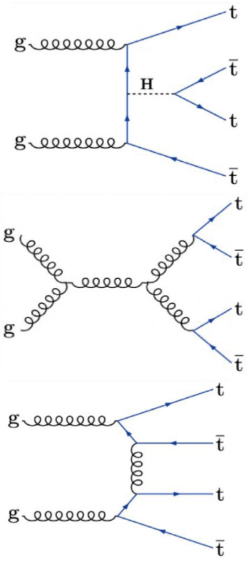
- Today's talk: DNN for reconstruction, final observable and future prospects

Search for $t\bar{t}t\bar{t}$ production

[CMS-TOP-21-005]

- Rare process in the SM
- Sensitive to top-Higgs coupling and new physics

→ **Important test of SM**



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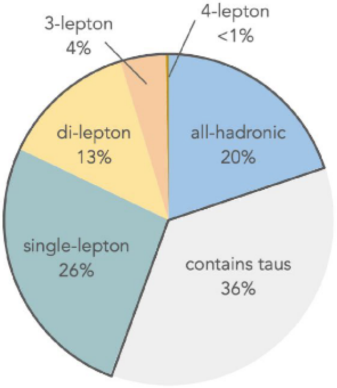
- Considered final states:
  - Single-lepton
  - Di-lepton (opposite/same sign)
  - **New: all-hadronic (all-had)**



M. Quinnan

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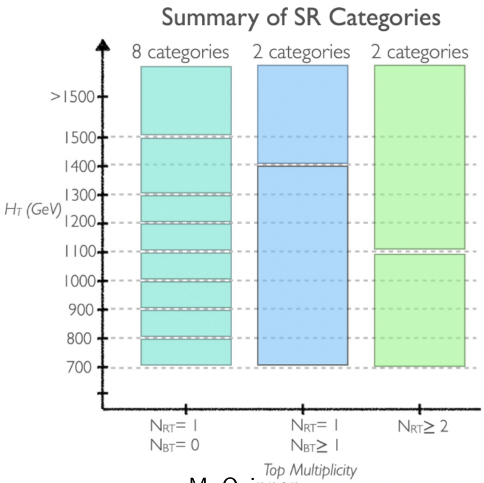
  - **New: all-hadronic (all-had)**
- **Strategy** in all-had channel
  - Selections: N(lepton) = 0, N(jets) $\geq$ 9, N(b-jets) $\geq$ 3, $H_T \geq 700$ GeV
  - Train **binary BDT** to separate signal vs. background
  - **Further separation** using tagged resolved tops (N_{RT}), tagged boosted tops (N_{BT}) and H_T



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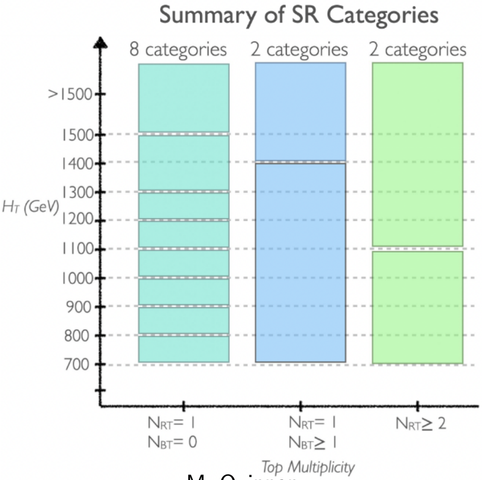
- **Challenge**: modeling of dominant backgrounds **$t\bar{t}$, QCD**

→ Use **extended ABCD** method



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Data-driven estimation in $t\bar{t}t\bar{t}$ all-had

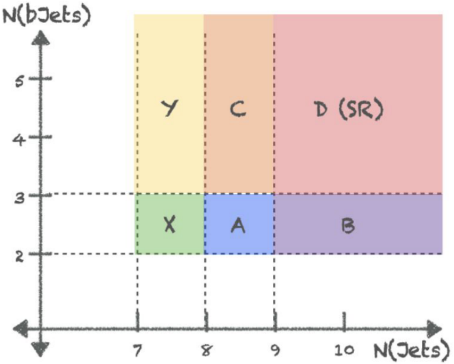
[CMS-TOP-21-005] [arXiv:2008.03636] [arXiv:1804.00779]

- Idea: use extended ABCD method for **data-driven estimation of $t\bar{t}$ and QCD**

$$D = \underbrace{\left(\frac{B \cdot C}{A}\right)}_{\text{ABCD}} \cdot \underbrace{\left(\frac{C \cdot X}{Y \cdot A}\right)}_{\text{higher-order terms}}$$

- Regions defined by **control variables** $\vec{c}$
- Works well for yield, but limited use of information

$\rightarrow$ Use **Neural Autoregressive Flow** (NAF) to estimate shape



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NAF for shape estimation

[CMS-TOP-21-005] [arXiv:2008.03636] [arXiv:1804.00779]

- **Goal:** learn transformation τ: $\mathcal{P} \to \mathcal{P}'$

$$\mathcal{P}'(\vec{x}'|\vec{c}') = \sum_{\vec{c}' \neq \vec{c}} \int \tau(\vec{x}'; \vec{x}|\vec{c}'; \vec{c}) \mathcal{P}(\vec{x}|\vec{c}) d\vec{x}$$

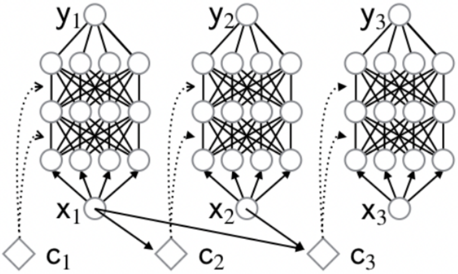
- **Basic principle**: use NAF as **universal approximator** for bijective transformations with sigmoidal function σ

$$y_d = f_t(x_t; \theta_t(\vec{c}, x_1, ..., x_{t-1})), \quad t = 1, ..., d$$

$$f_i(x_i; \theta_i) = \sigma^{-1}\left(w^{\mathsf{T}} \cdot \sigma(\vec{a}_i(\theta_i)x + \vec{b}_i(\theta_i))\right)$$

$$\Rightarrow \mathcal{P}'_{\text{target}}(\vec{x}'|\vec{c}') = \int \tau(\vec{x}'; \vec{x}|\vec{c}'; \vec{c}) \mathcal{P}_{\text{source}}(\vec{x}|\vec{c}) d\vec{x}$$

$$= \tau(\vec{x}'; \vec{x}|\vec{c}'; \vec{c}) \otimes \mathcal{P}_{\text{source}}(\vec{x}|\vec{c})$$



NAF in $\mathrm{t\bar{t}t\bar{t}}$ all-had analysis

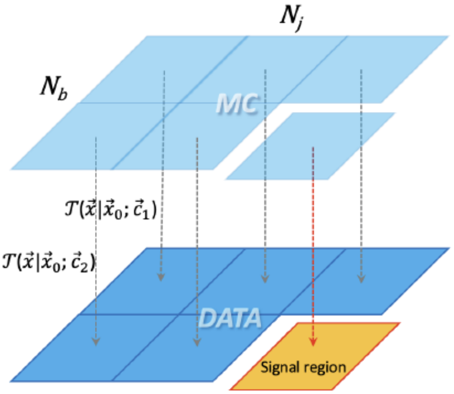
[CMS-TOP-21-005] [arXiv:2008.03636] [arXiv:1804.00779]

$$\mathcal{P}'_{\text{target}}(\vec{x}'|\vec{c}' = \tau(\vec{x}';\vec{x}|\vec{c}';\vec{c}) \otimes \mathcal{P}_{\text{source}}(\vec{x}|\vec{c})$$

- $\mathcal{P}'_{\text{target}}$: data – $\mathrm{t\bar{t}t\bar{t}}$ – minor backgrounds (simulation)
- $\mathcal{P}_{\text{source}}$: $\mathrm{t\bar{t}}$ simulation
- $\vec{x}$: H_T and BDT score
- Loss function: maximum-mean-discrepancy (MMD)
- Train **w/o SR**
- **Validation**: test method in orthogonal region (VR)

→ Construct uncertainty from observed differences

- **Apply in SR**



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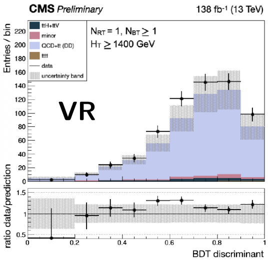

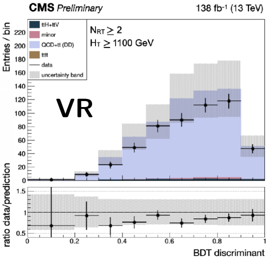

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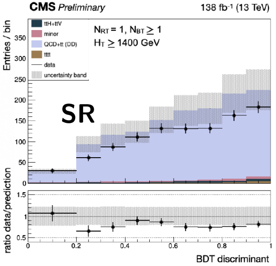
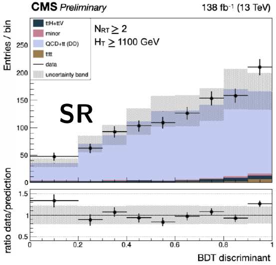
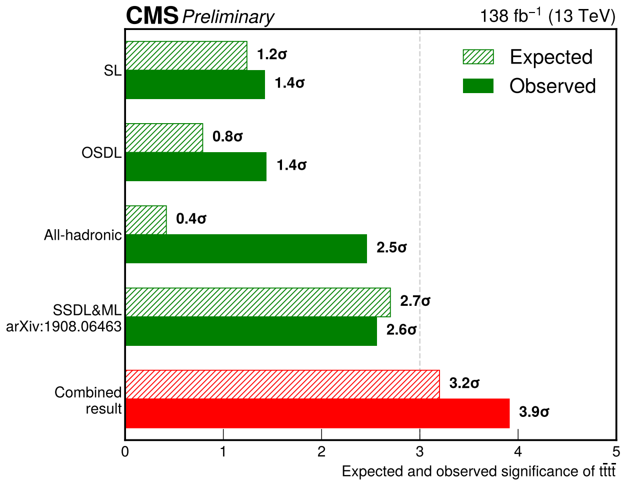
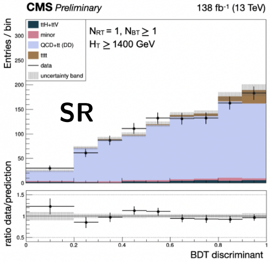


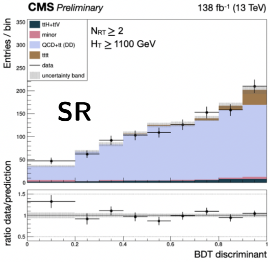


Results

[CMS-TOP-21-005]







EFT Analysis in associated Z production

[JHEP12(2021)083, CMS-TOP-21-001]

- Search for BSM physics in the scope of Effective Field Theory (EFT)

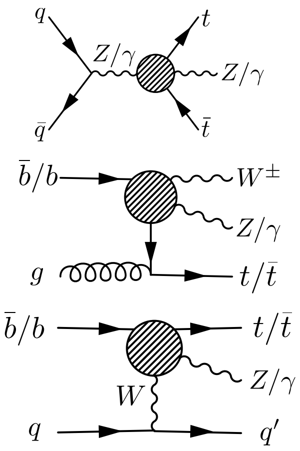
$$\mathcal{L}_{\mathrm{EFT}} = \mathcal{L}_{\mathrm{SM}} + \sum_{i}^{\mathrm{dim(6)}} \frac{c_i}{\Lambda^2}\mathcal{O}_i$$

- Targeting $t\bar{t} + Z$, tZW, tZq processes
- Considering EFT operators

$\mathcal{O}_{tZ}$, $\mathcal{O}_{tW}$	EWK dipole moments
$\mathcal{O}^{3}_{\varphi Q}$	left-handed SU(2) triplet current
$\mathcal{O}^{-}_{\varphi Q}$, $\mathcal{O}_{\varphi t}$	neutral current operators for left-(right-) handed top quarks

- Events distributed into five orthogonal regions: SR-3l, SR-4l, 2 control regions, 1 data-driven region

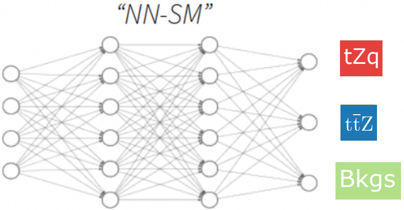
→ **New**: Considers interference effects **during** ML training!



[arXiv:1904.05637]

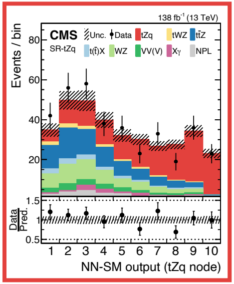
ML in CMS EFT analysis

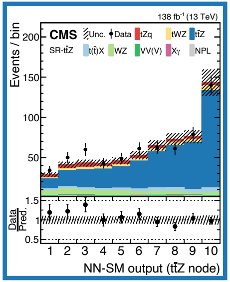
[JHEP12(2021)083, CMS-TOP-21-001]

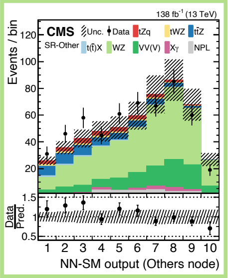


Inputs

Probability of hypothesis

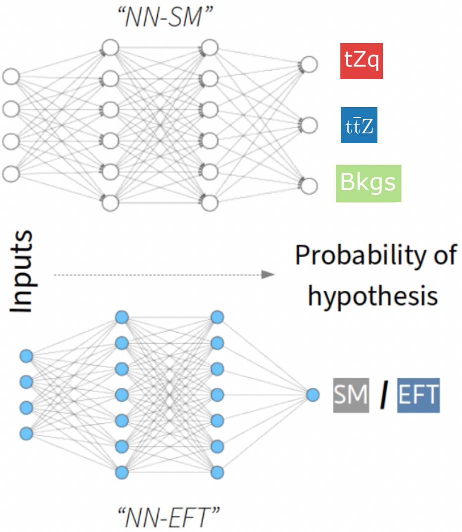






ML in CMS EFT analysis

[JHEP12(2021)083, CMS-TOP-21-001]



- Further trainings with events classified as tZq and $t\bar{t} + Z$

→ **Binary classification** of SM vs. EFT with following setups

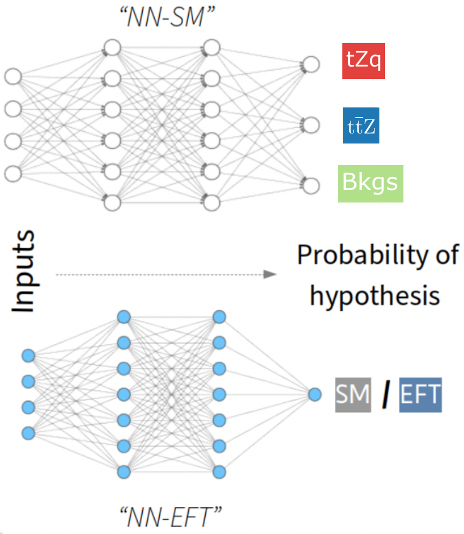
  1D: Consider only one operator at a time

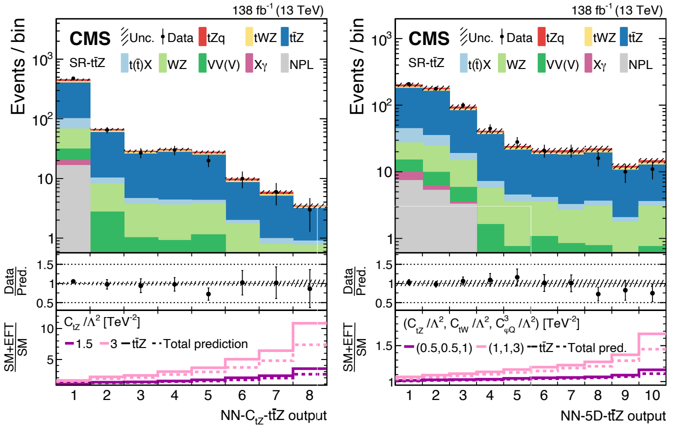
  5D: Consider effects from all operators simultaneously

⇒ Total of **8 EFT NNs**

ML in CMS EFT analysis

[JHEP12(2021)083, CMS-TOP-21-001]





Results

[JHEP12(2021)083, CMS-TOP-21-001]

WC/Λ^2 $[\text{TeV}^{-2}]$	95% CL confidence intervals			
	Other WCs fixed to SM		5D fit	
	Expected	Observed	Expected	Observed
c_{tZ}	$[-0.97, 0.96]$	$[-0.76, 0.71]$	$[-1.24, 1.17]$	$[-0.85, 0.76]$
c_{tW}	$[-0.76, 0.74]$	$[-0.52, 0.52]$	$[-0.96, 0.93]$	$[-0.69, 0.70]$
$c^{3}_{\varphi Q}$	$[-1.39, 1.25]$	$[-1.10, 1.41]$	$[-1.91, 1.36]$	$[-1.26, 1.43]$
$c^{-}_{\varphi Q}$	$[-2.86, 2.33]$	$[-3.00, 2.29]$	$[-6.06, 14.09]$	$[-7.09, 14.76]$
$c_{\varphi t}$	$[-3.70, 3.71]$	$[-21.65, -14.61] \cup [-2.06, 2.69]$	$[-16.18, 10.46]$	$[-19.15, 10.34]$

- Increase in sensitivity by usage of ML between 20-70 %

$\rightarrow$ **ML crucial for this analysis**

ML in Future Applications

Looking forward: Future applications of ML

- Modeling of underlying physics crucial for many top-related analyses

$\rightarrow$ Parameters in simulation programs (e.g. Pythia) crucial

- Many parameters not derivable from first principles, obtained with ambiguities
- Solution: Generate dedicated simulations with varied parameter values
- **Problem**: dedicated samples often have **limited statistics**, challenging to obtain meaningful uncertainty estimate

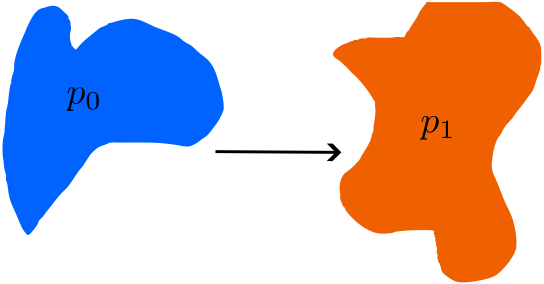
$\rightarrow$ Question: Can ML techniques help here?

Possible solution: DCTR approach

[PhysRevD.101.091901]

- Underlying problem: find transformation $p_0(x) \rightarrow p_1(x)$

$\rightarrow$ find $w(x) = p_0(x)/p_1(x)$



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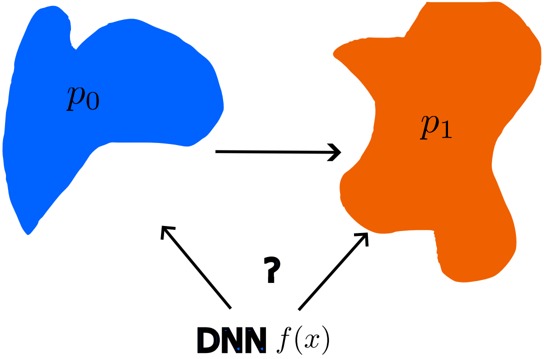
- Problem can be solved with ML

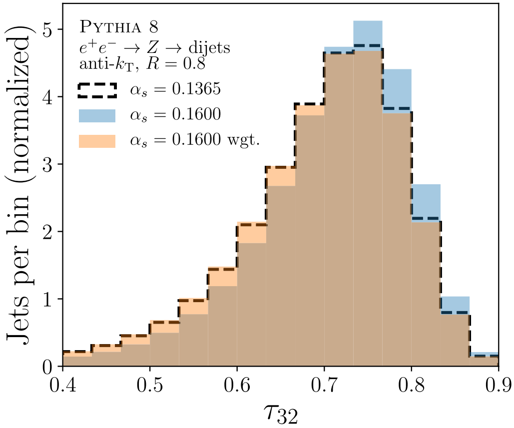
$$w(x) \sim \frac{f(x)}{1 - f(x)}$$



Advantages of DCTR

[PhysRevD.101.091901]

- Use **full, multidimensional** phase space for derivation of weights
- Enables **continuous weights** for whole phase space
- Can also be used for **derivation of the parameters** directly from data
- Approach already used in GAN application [JINST 15 P11004] and top-related analyses [JHEP09(2021)058]
- On-going study to check applicability



Conclusions

- ML has **significant role** in top physics!
- Wide array of strategies and applications, very **active field of research**
  - Reconstruction with **Neural Autoregressive Flows** [CMS-TOP-21-005]
  - Analysis with **full EFT effects in ML training** [JHEP12(2021)083, CMS-TOP-21-001]
- Many **new developments** on-going, e.g. **DCTR** [PhysRevD.101.091901]

$\rightarrow$ **Stay tuned!**

Backup

Systematic uncertainties in $t\bar{t}t\bar{t}$

[CMS-TOP-21-005]

Source	Uncertainty	Process	Final state	correlated (years)	correlated (Process)
Normalization only					
Luminosity	1–2%	All	All		✓
Electron Id/Isolation/Trigger	3%	All	OSDL+SL		✓
Muon Id/Isolation/Trigger	3%	All	OSDL+SL		✓
Modelling $t\bar{t}$ + HF	4–8%	$t\bar{t} + b\bar{b}$	OSDL+SL	✓	✓
ME-PS matching	+7.5%/-9.6%	$t\bar{t}$	OSDL		
Cross section $t\bar{t}$ +bb	+4.8%/-5.5%	$t\bar{t}$ +bb	OSDL+SL	✓	
Cross section $t\bar{t}$ +light jets	+4.8%/-5.5%	$t\bar{t}$ +light jets	OSDL+SL	✓	
Cross section TOP	4%	TOP	SL	✓	
Cross section $t\bar{t}$ +H	20%	$t\bar{t}$ H	All	✓	
Cross section $t\bar{t}$ +V	50%	$t\bar{t}$ V	OSDL	✓	
Cross section $t\bar{t}$ +rare	50%	$t\bar{t}$ Rare	OSDL	✓	
Cross section EWK	3.8%	EWK	OSDL+SL	✓	
Shape and Normalization					
Prefire	$\pm\sigma$	All	All, 2016+2017 only		
Pileup	$\sigma_{\text{minbias}} \pm 4.6\%$	All	All	✓	✓
Jet Energy Scale	$\pm\sigma(p_T, \eta)$	All	All		✓
Jet Energy Resolution	$\pm\sigma(\eta)$	All	All		✓
DeepCSV tagging	$\pm\sigma(p_T)$	All	SL		✓
DeepCSV tagging stats	$\pm\sigma$	All	SL		✓
DeepJet tagging	$\pm\sigma$	All	OSDL, hadronic		✓
DeepJet tagging stats	$\pm\sigma$	All	OSDL, hadronic		✓
resolved t tagging: statistical	$\pm\sigma$	All	SL, hadronic		
resolved t tagging: CS purity	$\pm\sigma(p_T)$	All	SL		
resolved t tagging: closure	$\pm\sigma(N_{jet})$	All	SL		
PDF	$\pm\sigma$	$t\bar{t}$	All	✓	✓
Renorm./Fact. Energy Scale	envelope($\times 2$, $\times 0.5$)	All	SL, hadronic	✓	
Renorm./Fact. Energy Scale	$\times 2$, $\times 0.5$	All	OSDL	✓	
Shape only					
ISR	$\pm\sigma$	All	All	✓	
FSR	$\pm\sigma$	All	All	✓	

Systematic uncertainties in $t\bar{t}t\bar{t}$ all-had

[CMS-TOP-21-005]

Name	Type	Processes	Correlations	$t\bar{t}t\bar{t}$ Signal Uncertainty (in percent)	Background Uncertainty (in percent)
Statistics of data-driven backgrounds	shape	QCD+$t\bar{t}$	-	-	5-30
Statistics of transformed samples	shape	QCD+$t\bar{t}$	-	-	10
Statistics of simulated samples	shape	$t\bar{t}t\bar{t}$, ttX, other	-	0-20	0-20
Data-prediction normalization	lnN	QCD+$t\bar{t}$	-	-	5-37
Data-prediction shape uncertainty	shape	QCD+$t\bar{t}$	-	-	n/a
DeepJet b-tag SF (HF, LF, cferr)	shape	$t\bar{t}t\bar{t}$, ttX, other	processes+years	0-10	0-10
DeepJet b-tag SF (stats)	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	0-10	0-10
Resolved top efficiency SF	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	0-5	0-5
Resolved top mistag SF	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	0-10	0-10
DeepAK8 boosted top SF	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	0-5	0-5
DeepAK8 boosted W SF	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	0-10	0-5
JER	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	0-20	0-20
JES	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	5-20	5-20
Pileup	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	0-5	0-5
Trigger efficiency	shape	$t\bar{t}t\bar{t}$, ttX, other	processes	0-5	0-5
Lepton veto	lnN	$t\bar{t}t\bar{t}$, ttX	processes	0-5	0-5
Luminosity	lnN	$t\bar{t}t\bar{t}$, ttX, other	processes	2.3-2.5	2.3-2.5
PDF	shape	$t\bar{t}t\bar{t}$, ttX	processes+years	0-10	0-10
ISR	shape	$t\bar{t}t\bar{t}$, ttX	years	0-5	0-5
FSR	shape	$t\bar{t}t\bar{t}$, ttX	years	0-20	0-20
μ_R, μ_F	shape	$t\bar{t}t\bar{t}$, ttX	years	0-20	0-20
Cross section	lnN	ttX	processes+years	-	26
Prefire	lnN	$t\bar{t}t\bar{t}$, ttX (2016, 2017)	processes	< 1	< 1

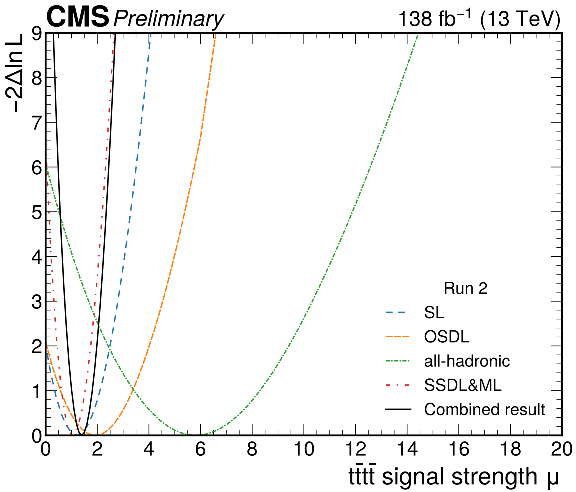
Results in $t\bar{t}t\bar{t}$

[CMS-TOP-21-005]

Analysis	Signal strength		Significance		Cross section
	exp	obs	exp	obs	obs (fb)
OSDL	$1^{+1.6}_{-1.6}$	$2.8^{+1.8}_{-1.6}$	0.6	1.8	37^{+21}_{-20}
Single lepton	$1^{+0.9}_{-0.8}$	$1.2^{+0.9}_{-0.9}$	1.2	1.4	15^{+13}_{-11}
All-hadronic	$1^{+2.5}_{-2.4}$	$5.8^{+2.5}_{-2.4}$	0.4	2.5	70^{+30}_{-29}
New results only	$1^{+0.7}_{-0.7}$	$2.5^{+0.7}_{-0.7}$	1.5	3.7	38^{+13}_{-11}
SSDL & multilepton [26]	$1^{+0.4}_{-0.4}$	$1.0^{+0.5}_{-0.4}$	2.7	2.6	13^{+6}_{-5}
All CMS 2016–2018	$1^{+0.4}_{-0.3}$	$1.4^{+0.4}_{-0.4}$	3.2	3.9	17^{+5}_{-5}

Negative Log Likelihood in $t\bar{t}t\bar{t}$

[CMS-TOP-21-005]



EFT coefficients

[JHEP12(2021)083, CMS-TOP-21-001]

Operator	WC	Mapping to Warsaw-basis coefficients
$\mathcal{O}_{\mathrm{tZ}}$	c_{tZ}	$\mathrm{Re}\{-s_{\mathrm{W}} c_{\mathrm{uB}}^{(33)} + c_{\mathrm{W}} c_{\mathrm{uW}}^{(33)}\}$
$\mathcal{O}_{\mathrm{tW}}$	c_{tW}	$\mathrm{Re}\{c_{\mathrm{uW}}^{(33)}\}$
$\mathcal{O}_{\varphi\mathrm{Q}}^{3}$	$c_{\varphi\mathrm{Q}}^{3}$	$c_{\varphi\mathrm{q}}^{3(33)}$
$\mathcal{O}_{\varphi\mathrm{Q}}^{-}$	$c_{\varphi\mathrm{Q}}^{-}$	$c_{\varphi\mathrm{q}}^{1(33)} - c_{\varphi\mathrm{q}}^{3(33)}$
$\mathcal{O}_{\varphi\mathrm{t}}$	$c_{\varphi\mathrm{t}}$	$c_{\varphi\mathrm{u}}^{(33)}$

Analysis selections

[JHEP12(2021)083, CMS-TOP-21-001]

Selection requirement	SR-3ℓ	SR-$t\bar{t}$Z-4ℓ	WZ CR	ZZ CR
Lepton multiplicity	=3	=4	=3	=4
$m_{3\ell} - m_{Z}$	—	—	>15 GeV	—
Z boson candidates multiplicity	=1	=1	=1	=2
Jet multiplicity	≥2	≥2	—	—
b jet multiplicity	≥1	≥1	=0	—
p_{T}^{miss}	—	—	>50 GeV	—

Input features

[JHEP12(2021)083, CMS-TOP-21-001]

Variable	NN-SM	NN-c_{tZ}-tZq	NN-c_{tZ}-t$\bar{t}$Z	NN-c_{tW}-tZq	NN-c_{tW}-t$\bar{t}$Z	NN-$c^{3}_{\varphi Q}$-tZq	NN-$c^{3}_{\varphi Q}$-t$\bar{t}$Z	NN-5D-tZq	NN-5D-t$\bar{t}$Z
p_{T}^{Z}	—	✓	✓	✓	✓	✓	✓	✓	✓
$\eta(Z)$	✓	✓	✓	—	—	✓	—	—	✓
$\Delta\phi(\ell_1^Z \ell_2^Z)$	✓	✓	✓	✓	✓	✓	✓	✓	✓
$p_T(t)$	✓	✓	✓	—	✓	✓	—	✓	✓
$\eta(t)$	—	✓	✓	✓	✓	✓	—	—	✓
$m(t, Z)$	—	—	—	—	—	—	—	—	—
$\lvert\eta(j')\rvert$	✓	—	—	—	—	—	—	✓	—
$p_T(j')$	✓	✓	—	✓	—	—	—	—	—
$\Delta R(b, \ell_t)$	—	✓	—	✓	—	—	—	—	—
$\Delta R(j', \ell_t)$	✓	—	—	—	—	—	—	—	—
$\Delta R(t, Z)$	—	✓	✓	✓	—	✓	—	—	✓
$\Delta\eta(Z, j')$	—	✓	—	—	—	—	—	✓	—
ΔR between t and the closest lepton	—	✓	—	✓	—	—	—	—	—
ΔR between j' and the closest lepton	—	—	—	—	—	—	—	✓	—
$m_{3\ell}$	✓	—	—	—	✓	—	✓	—	✓
m_T^W	✓	✓	✓	—	—	—	—	—	✓
p_T^{miss}	✓	—	—	—	—	—	—	—	—
Lepton asymmetry	✓	—	—	✓	✓	—	—	✓	—
$\cos\theta_Z^{\star}$	—	—	✓	—	—	✓	—	—	✓
Max. p_T among jet pairs	—	—	—	—	—	—	✓	—	✓
Max. DEEPJET discriminant	✓	—	—	—	—	—	—	—	—
b jet multiplicity	✓	—	—	—	—	—	—	—	—
Three-momenta of the three leading leptons	✓	—	—	—	—	—	—	—	—
Three-momenta of the three leading jets	✓	—	—	—	—	—	—	—	—
DEEPJET discriminants of the three leading jets	✓	—	—	—	—	—	—	—	—
Number of variables	33	11	8	8	6	7	4	7	10

Systematic uncertainties

[JHEP12(2021)083, CMS-TOP-21-001]

	Source	Type	Correlation
Experimental	Integrated luminosity	Yield	Partial
	Trigger efficiency	Yield	—
	Pileup	Both	✓
	Lepton identification and isolation	Both	✓
	b tagging	Both	Partial
	Jet energy scale	Both	Partial
	Jet energy resolution	Both	—
	Missing transverse momentum	Both	—
	L1 ECAL inefficiency	Both	✓
Theoretical	PDF	Both	✓
	α_S	Both	✓
	ME scales μ_R, μ_F	Both	✓
	Signal SM cross sections	Yield	✓
	ISR and FSR	Both	✓
	Additional radiation	Shape	✓
Backgrounds	WZ normalization	Yield	✓
	VV(V) normalization	Yield	✓
	$t(\bar{t})X$ normalization	Yield	✓
	$X\gamma$ normalization	Yield	✓
	NPL normalization	Yield	✓
	NPL misidentification probabilities	Both	✓

Observables for inference

[JHEP12(2021)083, CMS-TOP-21-001]

Fit configuration	Region					
	SR-tZq	SR-t$\bar{\text{t}}$Z	SR-Others	SR-t$\bar{\text{t}}$Z-4ℓ	CR WZ	CR ZZ
1D c_{tZ}	NN-c_{tZ}-tZq	NN-c_{tZ}-t$\bar{\text{t}}$Z	m_{T}^{W}	Counting experiments		
1D c_{tW}	NN-c_{tW}-tZq	NN-c_{tW}-t$\bar{\text{t}}$Z				
1D $c_{\varphi\text{Q}}^{3}$	NN-$c_{\varphi\text{Q}}^{3}$-tZq	NN-$c_{\varphi\text{Q}}^{3}$-t$\bar{\text{t}}$Z				
1D $c_{\varphi\text{Q}}^{-}$	NN-SM (tZq node)	NN-SM (t$\bar{\text{t}}$Z node)				
1D $c_{\varphi\text{t}}$	NN-SM (tZq node)	NN-SM (t$\bar{\text{t}}$Z node)				
2D and 5D	NN-5D-tZq	NN-5D-t$\bar{\text{t}}$Z				

Contribution of uncertainty groups

[JHEP12(2021)083, CMS-TOP-21-001]

Source	c_{tZ}	c_{tW}	$c^{3}_{\varphi Q}$	$c^{-}_{\varphi Q}$	$c_{\varphi t}$
tZq normalization	<0.1	<0.1	1.2	0.1	0.8
$t\bar{t}Z$ normalization	0.6	<0.1	0.4	37	38
tWZ normalization	0.1	0.1	<0.1	0.7	2.1
Background normalizations	<0.1	<0.1	6.9	3.6	6.8
NPL background estimation	1.4	0.2	5.6	0.3	3.8
Jet energy scale	<0.1	<0.1	0.8	0.7	2.3
Jet energy resolution	<0.1	<0.1	<0.1	<0.1	1.4
p_T^{miss}	<0.1	<0.1	<0.1	<0.1	0.2
b tagging	<0.1	<0.1	0.9	2.0	0.3
Other (experimental)	<0.1	<0.1	1.6	0.8	0.6
Lepton identification and isolation	0.4	0.4	1.2	2.2	0.8
Theory	2.1	1.1	0.4	0.9	0.9