# SEARCH FOR CHARGED-LEPTON FLAVOR VIOLATION IN THE PRODUCTION AND DECAY OF TOP QUARKS AT $\sqrt{S}=13$ TEV WITH THE CMS DETECTOR

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#### **Abstract**

A search for charged-lepton flavor violation has been performed in the top quark sector through both top quark production and decay signal processes. The data were collected by the CMS experiment from proton-proton collisions at a center-of-mass energy of 13 TeV and correspond to an integrated luminosity of 138 fb<sup>-1</sup>. The selected events are required to contain one opposite-sign electron-muon pair, a third charged lepton (electron or muon), at least one jet, and at most one jet associated with a bottom quark. The analysis utilizes boosted decision trees to separate background processes from a possible signal, exploiting differences in the kinematics of the final state particles. The data are found to be consistent with the standard model expectation. Upper limits at 95% confidence level are placed on the branching fractions involving up (charm) quarks,  $t \rightarrow e \mu u$  ( $t \rightarrow e \mu c$ ), of  $0.032 \times 10^{-6}$  ( $0.498 \times 10^{-6}$ ),  $0.022 \times 10^{-6}$  ( $0.369 \times 10^{-6}$ ), and  $0.012 \times 10^{-6}$  ( $0.216 \times 10^{-6}$ ) for tensor, vector, and scalar interactions, respectively.

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### List of Acronyms

AR application region

**ATLAS** A Toroidal LHC Apparatus

**BDT** Boosted Decision Tree

**CLFV** Charged-Lepton Flavor Violation

**CMS** Compact Muon Solenoid

**EFT** Effective Field Theory

**HLT** High Level Trigger

**HL-LHC** High Luminosity-LHC

LHC Large Hadron Collider

**LO** leading order

**L1** Level-1

MC Monte-Carlo

ME matrix-element

**MET** missing transverse momentum

MR measurement region

**MVA** multivariate analysis

NLO next-to-leading order

NN neural network

NNLO next-to-next-to-leading order

**OSDF** opposite-sign and different-flavor

**OSSF** opposite-sign and same-flavor

**PD** Primary Dataset

**PDF** Parton Distribution Function

**PF** particle flow

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PU pile-up

**PV** primary vertex

**QCD** quantum chromodynamics

**SM** Standard Model

**SR** signal region

**SSSF** same-sign and same-flavor

**SV** secondary vertex

**VR** validation region

**WC** Wilson Coefficient

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# Introduction

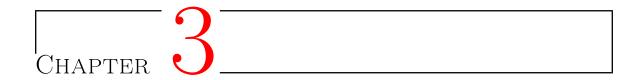
## Part I

# **Theoretical Framework**



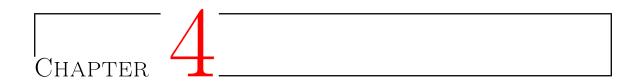
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- 2.2 Higgs Mechanism
- 2.3 Flavor Sector



### Beyond the Standard Model

- 3.1 Overview of the BSM Theories
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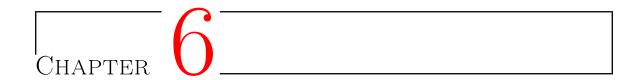


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## Part II

# **Experimental Apparatus**

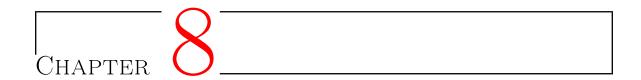


The Large Hadron Collider



### The Compact Muon Solenoid Detector

- 7.1 Coordinate System Used in the CMS Detector
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## Object Reconstruction in the CMS detector

- 8.1 Electron and Photon
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- **8.4** Jets
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### Run-3 Operation of the CMS detector

- 9.1 The CMS Run Organisation
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# Chapter 10

### The Phase-2 Upgrade of the CMS Detector

- 10.1 Overview of the Upgrade
- 10.2 Leve-1 Track Finder
- 10.3 Leve-1 Electron Trigger Algorithm

### Part III

# Search for Flavor-Violating eµtq Interactions

# Chapter 11

### **Previous searches**

- 11.1 ATLAS
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[1]

### Datasets, Simulated Samples and Triggers

This analysis is based on data collected by the Compact Muon Solenoid (CMS) experiment in 2016-2018 from pp collisions at a center-of-mass energy of 13 TeV corresponding to an integrated luminosity of 138 fb $^{-1}$ . There were approximately 30 simultaneous pp collisions occurring per 25 ns. Based on online selection criteria, fully reconstructed collision data that contain high-level physics objects are divided into "Primary Datasets (PDs)". The PDs that make use of lepton information for selection include "DoubleEG", "DoubleMu", "MuonEG", "SingleElectron", and "SingleMuon" for 2016 and 2017 data taking era. In 2018, "SingleElectron", "DoubleEG" are replaced by "EGamma". The names of these PDs reflect the selection criteria. In addition to these PDs, MC samples are also generated to model both signal and background processes, which are described in section 12.1 and section 12.2, respectively. To account for the different data taking conditions across the years, all MC samples are generated separately for each year. HLT triggers are used to select events offline, which is described in section 12.3.

#### 12.1 Signal Samples

In this analysis, New Physics is described by Dimension-6 Effective Field Theory (EFT) operators,

$$\mathcal{L} = \mathcal{L}_{SM}^{(4)} + \frac{1}{\Lambda^2} \sum_{a} C_a^{(6)} O_a^{(6)} + O\left(\frac{1}{\Lambda^4}\right). \tag{12.1}$$

Among many of the Dimension-6 operators in Warsaw basis [2], a total of 6 operators are considered, which are summarized in Table 12.1. To reduce the number of free parameters, the permutations of fermion flavors are combined. Taking eutu vertex as an example, the Wilson Coefficients (WCs) are parameterized in the following way:

$$\begin{array}{lll} C_{lq} & = & C_{lq}^{(1)1213} + C_{lq}^{(1)2113} + C_{lq}^{(1)1231} + C_{lq}^{(1)1213}, & (12.2) \\ C_{lu} & = & C_{lu}^{1213} + C_{lu}^{2113} + C_{lu}^{1231} + C_{lu}^{1213}, & (12.3) \\ C_{eq} & = & C_{eq}^{1213} + C_{eq}^{2113} + C_{eq}^{1231} + C_{eq}^{1213}, & (12.4) \\ C_{eu} & = & C_{eu}^{1213} + C_{eu}^{2113} + C_{eu}^{1231} + C_{eu}^{1213}, & (12.5) \end{array}$$

$$C_{lu} = C_{lu}^{1213} + C_{lu}^{2113} + C_{lu}^{1231} + C_{lu}^{1231},$$
 (12.3)

$$C_{eq} = C_{eq}^{1213} + C_{eq}^{2113} + C_{eq}^{1231} + C_{eq}^{1213},$$
 (12.4)

$$C_{eu} = C_{eu}^{1213} + C_{eu}^{2113} + C_{eu}^{1231} + C_{eu}^{1213},$$
 (12.5)

**Table 12.1:** Summary of relevant dimension-6 operators considered in this analysis. Here,  $\varepsilon$  is the two dimensional Levi-Civita symbol,  $\gamma^{\mu}$  the gamma matrix, and  $\sigma^{\mu\nu} = \frac{i}{2} [\gamma^{\mu}, \gamma^{\nu}]$ . The I and q denote left-handed doublets, whereas u and e denote right-handed singlets. The indices i and jare lepton flavor indices that run from 1 to 2 with  $i \neq j$ ; m and n are quark flavor indices with the condition that one of them is 3 and the other one is 1 or 2.

Lorentz Structure	Operator				
vector	$O_{lq}^{(1)ijmn}$	=	$(\bar{I}_{\it i}\gamma^\muI_{\it j})(\bar{q}_{\it m}\gamma_\muq_{\it n})$		
	$O_lu^{ijmn}$	=	$(\bar{I}_i \gamma^\mu I_j) (\bar{u}_m \gamma_\mu u_n)$		
	$O_{eq}^{ijmn}$	=	$(\overline{\mathbf{e}}_i \gamma^{\mu} \mathbf{e}_j)(\overline{\mathbf{q}}_m \gamma_{\mu} \mathbf{q}_n)$		
	$O_{eu}^{ijmn}$	=	$(\overline{\mathrm{e}}_{i}\gamma^{\mu}\mathrm{e}_{j})(\overline{\mathrm{u}}_{m}\gamma_{\mu}\mathrm{u}_{n})$		
scalar	O <sub>lequ</sub>	=	$(\bar{I}_ie_j)\;\varepsilon\;(\overline{q}_mu_n)$		
tensor	$O_{lequ}^{(3)ijmn}$	=	$(\bar{I}_i\sigma^{\mu\nu}e_j)\;\varepsilon\;(\overline{q}_m\sigma_{\mu\nu}u_n)$		

$$C_{\text{lequ}}^{(1)} = C_{\text{lequ}}^{(1)1213} + C_{\text{lequ}}^{(1)2113} + C_{\text{lequ}}^{(1)1231} + C_{\text{lequ}}^{(1)1231}, \qquad (12.6)$$

$$C_{\text{lequ}}^{(3)} = C_{\text{lequ}}^{(3)1213} + C_{\text{lequ}}^{(3)2113} + C_{\text{lequ}}^{(3)1231} + C_{\text{lequ}}^{(3)1231}. \qquad (12.7)$$

$$C_{\text{leau}}^{(3)} = C_{\text{leau}}^{(3)1213} + C_{\text{leau}}^{(3)2113} + C_{\text{leau}}^{(3)1231} + C_{\text{leau}}^{(3)1213}.$$
 (12.7)

Additionally, all vector-like operators are combined,

$$O_{\text{e}\mu\text{tu}}^{\text{vector}} = O_{\text{lq}} + O_{\text{lu}} + O_{\text{eq}} + O_{\text{eu}}, \tag{12.8}$$

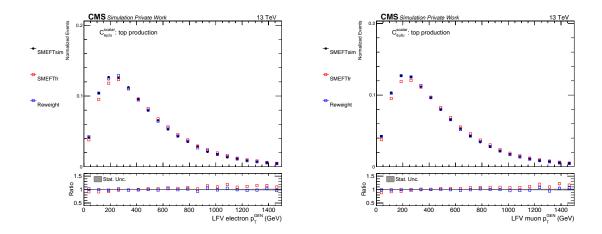
$$\begin{array}{lll} \mathsf{O}_{\mathsf{e}\mu\mathsf{t}\mathsf{u}}^{\mathsf{vector}} &=& \mathsf{O}_{\mathsf{l}\mathsf{q}} + \mathsf{O}_{\mathsf{l}\mathsf{u}} + \mathsf{O}_{\mathsf{e}\mathsf{q}} + \mathsf{O}_{\mathsf{e}\mathsf{u}}, & (12.8) \\ \mathsf{O}_{\mathsf{e}\mu\mathsf{t}\mathsf{u}}^{\mathsf{scalar}} &=& \mathsf{O}_{\mathsf{l}\mathsf{e}\mathsf{q}\mathsf{u}}^{(1)} + \mathsf{h.c.} & (12.9) \end{array}$$

$$O_{\text{e}\mu tu}^{\text{tensor}} = O_{\text{leq}u}^{(3)} + \text{h.c,}$$
 (12.10)

which results in 6 independent WCs:  $C_{e\mu tu}^{vector}$ ,  $C_{e\mu tu}^{scalar}$ ,  $C_{e\mu tu}^{tensor}$ ,  $C_{e\mu tc}^{vector}$ ,  $C_{e\mu tc}^{scalar}$ ,  $C_{e\mu tc}^{tensor}$ .

To generate signal MC samples, the effective Lagrangian described above is implemented using the SmeftFR v2 [3] model, and saved in the "UFO" format [4]. Additionally, all the WCs are set to 1 with  $\Lambda = 1$  TeV in the UFO, which then interfaces with the FEYNRULES [5] package to calculate Feynman diagrams. The output of the FEYNRULES is used in ME event generator MADGRAPH5 AMC@NLO v2.4.2 [6] to generate events at leading order (LO).

In general, the calculations done by the ME event generators are model-agnostic assuming the same EFT configurations. In other words, models like SmeftFR or SMEFTsim [7] are expected to give the same or very similar results in terms of cross sections and four-momenta of final-



**Figure 12.1:** Comparison of kinematic distributions at ME-level produced by different models: LFV electron  $p_T$  (left), LFV muon  $p_T$  (right). The "SmeftFR" samples (shown in red curve) and "SMEFTsim" samples (shown in black curve) are statistically independent of each other. The "Reweight" (shown in blue curve) are produced by applying weights calculated by Equation 12.11 to "SmeftFR" samples.

state particles. Nevertheless, visible differences in kinematics have been observed and shown in Figure 12.1. Furthermore, the cross sections predicted by SmeftFR v2 also yield more than 20% difference relative to SMEFTsim due to a bug that was later fixed in SmeftFR v3. In the light of these differences, the CMS and A Toroidal LHC Apparatus (ATLAS) Collaborations agreed to adopt the SMEFTsim model as the common standard. To quantify the impact of the choice of models on kinematics, the following ratio is calculated for each event *i*,

$$R_{\text{reweight}}^{i} = \frac{\omega_{\text{SMEFTsim}}^{i}}{\omega_{\text{SmeftFR}}^{i}},$$
(12.11)

where  $\omega_X^i$  is the per-event ME weight calculated by MADGRAPH5\_AMC@NLO using model X. Since SMEFTsim was not used by CMS at the time when the signal samples were generated,  $R_{\text{reweight}}$  are used to "reweight" the original samples generated using SmeftFR.

Due to the significant differences in kinematic distributions between top decay and production signals, MC samples are generated separately for these processes. The cross sections for top production signals are taken directly from  $MADGRAPH5\_AMC@NLO$  with SMEFTsim UFO as input. The event generation for top decay signals at the ME-level take two steps: (i) production of the SM  $t\bar{t}$ , and (ii) CLFV decay of one of the top quarks. Therefore, the  $t\bar{t}$  cross section at next-to-next-to-leading order (NNLO) precision [8] is used to normalize the top decay signals,

$$\sigma_{\rm CLFV}^{\rm Top\ Decay} = 2 \times \sigma_{\rm t\bar{t}}^{\rm NNLO} \times \mathcal{B}({\rm t} \rightarrow {\rm e\mu q}), \eqno(12.12)$$

where q={u,c}, and  $\mathcal{B}(t\to e\mu q)$  [9] can be expressed as,

$$\mathcal{B}(t \rightarrow e\mu q) = \frac{\frac{|C_{e\mu tq}^{vector}|^2}{\Lambda^4} \frac{m_t^5}{384\pi^3 \Gamma_t^{SM}}}{\frac{|C_{e\mu tq}^{scalar}|^2}{\Lambda^4} \frac{m_t^5}{3072\pi^3 \Gamma_t^{SM}}}{\frac{|C_{e\mu tq}^{tensor}|^2}{\Lambda^4} \frac{m_t^5}{64\pi^3 \Gamma_t^{SM}}}$$

$$(12.13)$$

where  $m_t$  and  $\Gamma_t^{SM}$  are taken to be 172.5 GeV and 1.33 GeV in this analysis, respectively. The choice of u or c quark in final states does not affect the cross sections of the top decay signals. The cross sections for all signal MC samples are summarized in Table 12.2.

**Table 12.2:** Theoretical cross sections for top production and decay for each CLFV coupling, calculated at  $C/\Lambda^2=1$  TeV<sup>-2</sup>. Uncertainties related to PDF and QCD scale in ME calculation are given  $(\sigma_{-\text{scale}}^{+\text{scale}} \pm \text{PDF})$ .

Lorentz Structure	Samples	XS (fb)	
vector	top production via u quark	$460^{+81}_{-64}\pm 6$	
	top production via c quark	$33^{+5}_{-4}\pm 6$	
	top decay via u/c quark	$32^{+0.8}_{-1.1}\pm1.3$	
scalar	top production via u quark	$97^{+18}_{-14}\pm1$	
	top production via c quark	$6.3^{+0.9}_{-0.8}\pm1.4$	
	top decay via u/c quark	$4.0^{+0.1}_{-0.1}\pm0.2$	
tensor	top production via u quark	$2143^{+368}_{-293}\pm31$	
	top production via c quark	$164^{+22}_{-18}\pm27$	
	top decay via u/c quark	$187^{+5}_{-6}\pm 8$	

Steps other than the ME calculation concerning signal MC generation follow the CMS standard, which is described in the following section.

### 12.2 Background Samples

Besides tZq, tHq, tHW, and tWZ processes, the next-to-leading order (NLO) Parton Distribution Function (PDF) set from NNPDF3.0 [10] is used in 2016 to generate background MC samples. The NNLO PDF set from NNPDF3.1 [11] is used for tZq while the LO PDF set from NNPDF3.0

**Table 12.3:** Summary of the configurations of the MC samples. DYM50 (DYM10to50) denote DY sample with a dilepton invariant mass greater than 50 GeV (between 10 and 50 GeV). V includes W and Z bosons. The cross sections for samples without a citation are taken directly from their event generators.

Category	Process	Event Generator	Perturbative QCD	Tune	XS precision
<i>prompt</i> background	WZ	MadGraph	NLO	CUETP8M1(CP5)	NLO [16]
	ZZ	POWHEG	NLO	CUETP8M1(CP5)	NLO [16]
	VVV	MadGraph	NLO CUETP8M1(CP5)		NLO
	$t\bar{t}W$ , $t\bar{t}Z$	MadGraph	NLO	CUETP8M1(CP5)	NLO [17, 18]
	tŧH	POWHEG	NLO	CUETP8M1(CP5)	NLO [18]
	tZq	MadGraph	NLO	CP5	NLO
	tHq, tHW, tWZ	MadGraph	LO	CUETP8M1(CP5)	LO
nonprompt background	tŧ	POWHEG	NLO	CUETP8M1(CP5)	NNLO [8]
	DYM50	MadGraph	NLO	CUETP8M1(CP5)	NNLO [19]
	DYM10to50	MadGraph	LO	CUETP8M1(CP5)	NLO [19]

is used for tHq, tHW, and tWZ in 2016. In 2017 and 2018, the NNLO PDF set from NNPDF3.1 is used to generate all the samples.

The default choice of ME event generator is MadGraph5\_AMC@NLO v2.4.2 (v2.2.2 for 2016), which is used to generate all but ZZ, tth, and tt samples. These three samples are generated with POWHEG v2 [12] instead. Samples with small contributions (thq, tWZ, thW, and low mass DY) are generated at LO while other samples are generated at NLO. Whenever possible and relevant, theoretical cross sections from high-order quantum chromodynamics (QCD) calculations are used. The references of these calculations are included in 12.3.

The PYTHIA v8.2 [13] is used to model parton shower and hadronization. The CUETP8M1 [14] is used in 2016 for underlying event tuning while the CP5 [15] is used in 2017 and 2018. The configurations of the MC samples are summarized in Table 12.3. The background processes are divided into two categories: (i) processes with three or more *prompt* leptons in the final states are classified as "*prompt* background", and (ii) other processes are classified as "*nonprompt* background". The *nonprompt* backgrounds in this analysis are modeled with a data-driven technique, which is discussed in chapter 15. The MC samples listed in "*nonprompt*" category in Table 12.3 are therefore only used for the purpose of validations.

### 12.3 Triggers

The target final states of this analysis contain three prompt leptons, which make lepton triggers the most optical choice to select events. To achieve the maximum acceptance, a combination of single-lepton, di-lepton and tri-lepton triggers are used. These triggers are summarized in Appendix A. Events in simulated samples are required to fire at least one of the triggers listed in Table A.1-A.3. Since multple PDs are used to record data events and the orthogonality of these PDs are not guaranteed by the online selection criteria, the following trigger logic is implemented to remove the overlap between different PDs:

- Events in SingleMuon datasets are required to fire at least one of the triggers listed under "SingleMuon".
- Events in DoubleMuon datasets are required to fire at least one of the triggers listed under "DoubleMu". Events are removed if they also fire at least one of the triggers listed under "SingleMuon".
- Events in MuonEG' datasets are required to fire at least one of the triggers listed under "MuonEG". Events are removed if they also fire at least one of the triggers listed under "SingleMuon" or "DoubleMu".
- Events in Single Electron datasets are required to fire at least one of the triggers listed under "SingleElectron". Events are removed if they also fire at least one of the triggers listed under "SingleMuon" or "DoubleMu" or "MuonEG".
- Events in DoubleEG datasets are required to fire at least one of the triggers listed under "DoubleEG". Events are removed if they also fire at least one of the triggers listed under "SingleMuon" or "DoubleMu" or "MuonEG" or "SingleElectron".
- Events in EGamma datasets are required to fire at least one of the triggers listed under "EGamma". Events are removed if they also fire at least one of the triggers listed under "SingleMuon" or "DoubleMu" or "MuonEG".

# Chapter 13

### **Object Selection**

Objects described in chapter 8, referred to as "candidates", are further selected with more stringent requirements with the goal of suppressing the contributions from background processes while maintaining a high signal acceptance. In particular, prompt electron and muon candidates are identified through a custom-trained Boosted Decision Tree (BDT) classifier, which is discussed in section 13.1. Two jet identification algorithms are deployed to select jet candidates originating from hard collisions, which is discussed in section 13.2. Furthermore, jet candidates that originate from b quarks are identified with a neural network (NN) based algorithm, which is discussed in section 13.3.

### 13.1 Lepton Selection

The target final states of this analysis feature exactly three leptons that originate either from decays of electroweak bosons or from the CLFV interaction, which in this analysis is a contact interaction that involves four fermions. These leptons, referred to as *prompt* leptons, typically appear to be isolated and not far away from the primary vertex (PV). In contrast, *nonprompt* leptons are leptons that originate from decays of hadrons, or from photon conversions, or misidentified leptons. They often travel a noticeable distance away from the PV and appear to be less isolated due to nearby activities. Due to the high multiplicity of leptons in our selection, backgrounds with at least one *nonprompt* lepton outnumber any other SM processes that produce three or more *prompt* leptons. It is therefore crucial to exploit the differences between *nonprompt* and *prompt* leptons and bring the *nonprompt* background under control.

#### 13.1.1 TOP LeptonMVA

The TOP LEPTONMVA is an offline lepton identification algorithm that is originally developed for tZq analyses [20, 21]. It is based on Gradient BDT implemented using the TMVA package [22]. A total of 13 features are used as input to the BDT. They can be categorised into four groups: (i) positions and momenta of the lepton candidates, (ii) isolation variables, (iii) variables associated to the closest jet, and (iv) a quality variable that is specific to electron or muon candidate. The version of TOP LEPTONMVA used by this analysis is the same as [21], where a detailed description of all input features can be found.

*Prompt* leptons from  $t\bar{t}W$ ,  $t\bar{t}Z$ , and tZq samples are used as signals in the BDT training while nonprompt leptons from  $t\bar{t}$  samples are used as backgrounds. The trained BDT outputs a single score for each lepton candidate ranging from -1 to 1 with -1 (1) being the most background-(signal-) like. the tight working point with a threshold of (>) 0.9 is chosen as the selection criteria for both electron candidates and muon candidates, which corresponds to a signal(background) efficiency of 90%(1%). The strategy is to trade a small percentage (<10%) of signal efficiency for several factors of background rejection.

#### 13.1.2 Full Selection

In addition to the TOP LEPTONMVA requirement, a set of common selection criteria are applied to both electron and muon candidates. The minimum  $p_{\rm T}$  requirement is 38GeV, 20 GeV, and 20 GeV for the leading, sub-leading, and trailing lepton in  $p_{\rm T}$ , respectively. This requirement is driven by the  $p_{\rm T}$  thresholds of the HLT triggers to avoid inefficiency at turn-on. Electron and muon candidates are required to be in the pseudorapidity range  $|\eta| < 2.4$ , which corresponds to the acceptance of CMS tracker and muon system in 2016-2018. The transverse (longitudinal) impact parameters with respect to the PV, denoted as  $d_{\rm xy}$  ( $d_{\rm z}$ ), is required to be in the range  $|d_{\rm xy}| < 0.05$  cm ( $|d_{\rm z}| < 0.05$  cm). The significance of the 3-dimensional impact parameter, denoted as SIP<sub>3</sub>, is defined as the 3-dimensional impact parameter divided by its uncertainty. It is required that SIP<sub>3</sub> < 8. The three cuts on impact parameters are added due to the difference in distributions of these parameters between *prompt* and *nonprompt* leptons. Also, they are part of the pre-selection requirement in the BDT training.

Furthermore, all lepton candidates are required to be isolated. This is achieved by first defining a cone with a distance parameter of  $\Delta R$  around each lepton candidate, where  $\Delta R = \sqrt{\Delta \eta^2 + \Delta \phi^2}$ . Only particles within  $\Delta R < R_{\text{max}}$  can contribute to the isolation variable, where  $R_{\text{max}}$  is referred to as the size of the cone. Secondly, a particle flow (PF) based isolation variable is defined as,

$$I_{\mathsf{mini}}^{\mathsf{rel}} = \frac{1}{\rho_{\mathsf{T}}^{\ell}} \{ \sum_{\mathsf{charged}} p_{\mathsf{T}} + \mathsf{max}(0, \sum_{\mathsf{neutral}} p_{\mathsf{T}} - \rho \mathcal{A}[\frac{\Delta R}{0.3}]^2) \}, \tag{13.1}$$

where  $p_T^\ell$  is the  $p_T$  of the lepton candidate, the first term inside the curly braces is the scalar sum of all charged particles associated with the PV while the second term evaluates the contribution from neutral particles. This is done by first scalar-summing over  $p_T$  of all neutral particles associated to the PV. A correction term, known as effective area correction [23], is then subtracted. This term is used to mitigate the impact of pile-up (PU) interactions. The size of the cone scales with  $p_T^\ell$  as,

$$R_{\rm max} = {\rm max}(0.05, {\rm min}(0.2, {10 {\rm GeV} \over p_{\rm T}^\ell})).$$
 (13.2)

.

This type of isolation variable is known as "mini" isolation, which maximises the signal efficiency at  $p_{\rm T}^\ell$  by reducing the cone size. It is required that lepton candidates to have  $I_{\rm mini}^{\rm rel} < 0.12$ .

For electron specifically, candidates are required to have a GSF track with one of less missing inner hit. Electron candidates reconstructed in the transition region between ECAL barrel and endcap (i.e.  $1.44 < |\eta_{SC}| < 1.57$ ) are removed from consideration. For muon specifically, candidates are required to be PF muons and pass the medium working point discussed in section 8.2.

Lepton candidates that pass all requirements stated above are referred to as "tight" leptons. Leptons selected with a separate set of criteria, known as "loose", is used in estimating the nonprompt background, which is discussed in chapter 15. Unless explicitly stated, all lepton objects presented in this search are tight leptons.

The energy of electron candidates are calibrated through. The moment scale of muon candidates are calibrated for muon candidates with  $p_{\rm T} < 200$  GeV. Scale factors are applied to *tight* leptons to correct for the differences in reconstruction, isolation, and identification between data and MC. These scale factors are obtained using dilepton events in Z resonance window.

### 13.2 Jet Selection

Jet candidates are reconstructed from PF candidates using the anti- $k_{\rm T}$  algorithm described in section 13.2 with a cone size of 0.4. Charged hadrons that are not associated to the PV are removed. Jet candidates are required to have a minimum  $p_{\rm T}$  of 30 GeV and in in the pseudorapidity range  $|\eta| < 2.4$ , where b-tagging are still effective. It is further required that all jet candidates to be isolated from *tight* leptons. A cone of the size 0.4 around each jet candidate is defined and candidates will be removed if any *tight* leptons are found within such a cone. This procedure is implemented to remove the overlap between leptons and jets.

The two primary sources of background are (i) detector noise, and (ii) jets from PU interactions. To suppress detector noise, a set of cut-based selections are applied to jet candidates. This algorithm utilizes information from PF candidates, including: (i) fraction of charged (neutral) hadrons energy, (ii) fraction of charged (neutral) EM energy, (iii) fraction of muon energy, and (iv) object multiplicity. The "tightLepVeto" working point is chosen to select jet candidates, which corresponds to 98-99% signal efficiency.

The second algorithm is designed to reject jet candidates that originate from PU interactions. This algorithm is based on a BDT that utilizes: (i) the trajectories of tracks associated to the jets, (ii) the topology of the jet shape, and (iii) object multiplicity. The *loose* working point is chosen to select jet candidates with  $p_{\rm T} < 50$  GeV, which corresponds to 99% signal efficiency. Applying this algorithm to jet candidates with  $p_{\rm T} > 50$  GeV is both ineffective and unnecessary as PU jets mostly reside in low  $p_{\rm T}$  spectrum. The overall effect of this algorithm on this analysis is small as PU jets constitute only a small fraction of all jet candidates in the phase space of this analysis.

As discussed in section 8.4, the energy scale for all jet candidates (data and MC) are calibrated. One extra correction is applied to simulated jets to recreate the jet energy resolution as measured in data.

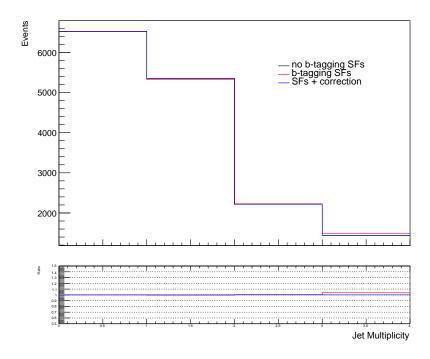
### 13.3 Identification of b jets

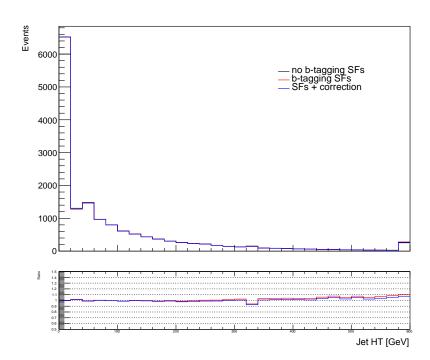
The DEEPJET algorithm [24] is used to identify jets that originate from b quark. The core strategy of this algorithm is to minimise information. This is achieved by removing entirely the selection of jet constituents, which limits the number of jet constituents considered. Additionally, an effort is made to use as many low-level features as possible, which further further deepens the feature space. Approximately a total of 650 input features are used, which can be categorized into four groups: (i) global variables, (ii) charged PF candidate features, (iii) neutral PF candidate features, (iv) and secondary vertex (SV) features associated with the jet. When compared to the existing DEEPCSV algorithm [25], DEEPJET algorithm delivers up to 20% improvement in signal efficiency while maintaining the same background efficiency.

The DEEPJET algorithm outputs a score ranging between 0 and 1, with 0 (1) being the most background- (signal-) like. The medium working point is chosen to tag b jet candidate, which corresponds to 70%-80% signal efficiency. The shape of the DEEPJET output distribution is corrected for the differences between data and MC in signal and background efficiencies. The per-event correction weight  $\omega$  is defined as,

$$\omega = \prod_{i}^{N_{\text{jets}}} SF(p_{T_i}, \eta_i, F_i, D_i), \qquad (13.3)$$

where SF is the ratio of efficiency in data to efficiency to MC parameterized as a function of  $p_T$ ,  $\eta$ , (MC truth) flavor F, as well as DEEPJET output D of each jet in the event.  $\omega$  is applied to all MC events, and additional scale factors are also applied to remove the normlization effect of  $\omega$ . These scale factors are measured using MC in e $\mu\ell$  channel described in chapter 14. The effect of these scale factors are shown in Figure 13.1.





**Figure 13.1:** Simulated events in  $e\mu\ell$  channel: jet multiplicity (top) and  $H_T$  (bottom).

# Chapter 14

### **Event Selection**

Events are required to contain exactly three tight leptons described in section 13.1. Furthermore, events are selected with HLT triggers discussed in section 12.3. Events with different lepton flavor composites are further categorized into three exclusive channels: eee,  $\mu\mu\mu$ ,  $e\mu\ell$ . In all three channels, the sum of the electric charges of the selected leptons are required to be 1 or -1. The leading leptons in all selected events are required to be matched with trigger objects within  $\Delta R < 0.2$ . Within each channel, different regions are defined to further understand signal and background.

eμ $\ell$  is the channel where close to 100% of the simuated signal events reside. This channel is divided into signal-enriched SRs and signal-depleted VRs, which are discussed in section 14.1 and section 14.2, respectively. Due to the lack of different flavors, the eee and μμμ channels are signal-depleted by definition. Therefore, events found in these two channels are only used to study background processes, which are discussed in section 14.2. The kinematic reconstruction of heavy particles, such as the top quark, is described in section 14.3.

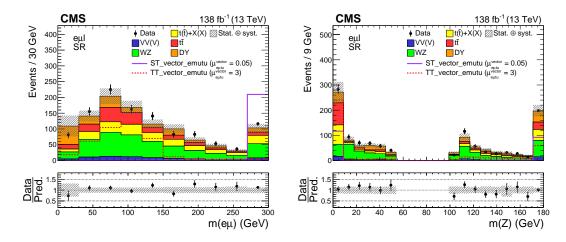
## 14.1 Signal Region

The core feature of the signal events is the presence of the "LFV e $\mu$ " pair, which consists of a pair of opposite-sign and different-flavor (OSDF) leptons. It is guaranteed that there is at least one OSDF pair in all events residing in e $\mu\ell$  channel due to the requirement on electric charges. The OSDF pair is immediately labelled as the LFV e $\mu$  pair if it is only possible to reconstruct one OSDF pair. In events where a pair of same-sign and same-flavor (SSSF) leptons are present, a kinematic reconstruction is used to determine which one of two leptons form the LFV e $\mu$  pair with the third lepton, which is detailed in section 14.3. Leptons that form the LFV e $\mu$  pair are referred to as the LFV electron or muon as it is assumed that they originate from the CLFV interaction. Based on the event topology of the signal process, further selection criteria are applied to define the SR. These selection criteria help achieve an optimal signal to background ratio by removing majority of the background events present in e $\mu\ell$  channel.

At tree-level, signal events are expected to contain one or two jets, which motivates a requirement of at least one jet in SR. Furthermore, it is required that there is no more than one b-tagged

jet to suppress the contribution from  $t\bar{t}$  events. Another prominent background is Drell-Yan production that features an OSSF pair. To suppress Drell-Yan processes in SR, events that contain an OSSF lepton pair with an invariant mass between 50 GeV and 106 GeV are removed. The lower bound of the this veto is lower than the typical value (e.g. 75 GeV) because the mass range between 50 GeV and 75 GeV has very few signal events and is dominated by *nonprompt* background from photon conversion. Additionally, a modest threshold of 20 GeV is applied to MET due to the presence of neutrinos in the signal events.

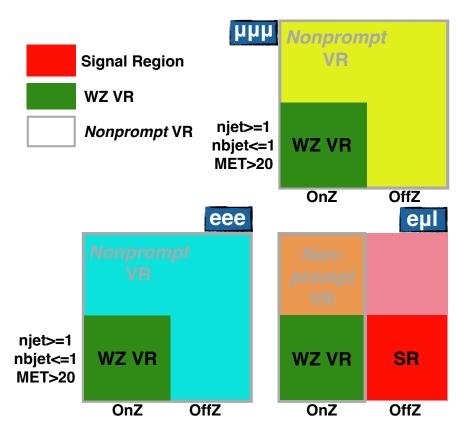
Distributions of the LFV e $\mu$  mass and the Z boson mass are shown in Figure 14.1. All backgrounds in Figure 14.1 are estimated using MC simulation even though strategy is to use a data-driven method to estimate the *nonprompt* background. This serves as a preliminary check to understand the components of different backgrounds in SR. Distributions of more variables in SR are included in Appendix B.



**Figure 14.1:** Distributions of the LFV e $\mu$  mass (left) and the Z boson mass (right) in SR. The data are shown as filled points and the SM background predictions as histograms. The VV(V) background includes ZZ and triboson production, while the  $t\bar{t}+X(X)$  component includes  $t\bar{t}W$ ,  $t\bar{t}Z$ ,  $t\bar{t}H$ , tZq, and smaller backgrounds containing one or two top quarks plus a boson or quark. All backgrounds are estimated using MC simulation. The hatched bands indicate statistical and systematic uncertainties for the SM background predictions. The normalisation of the signal processes is chosen arbitrarily for improved visualisation. The last bin of both histograms includes the overflow events.

Using the LFV  $e\mu$  mass, the SR is further divided into two subsets to create top production and decay enriched regions:

- SR1,  $m_{eu}$  < 150 GeV: top decay enriched.
- SR2, m<sub>eμ</sub> > 150 GeV: top production enriched.



**Figure 14.2:** Illustration of selection criteria used to define different regions. "OnZ" means the presence of at least one OSSF pair with an invariant mass between 50 GeV and 106 GeV. Events are labelled as "OffZ" when they fail "OnZ" criteria.

## 14.2 Validation Region

There are two types of signal-depleted VR defined across three channels: nonprompt VR and WZ VR. The purpose of these two types of VR is only limited to the validation of the background modelling as neither of them enter the final fit. It is expected that the nonprompt VR has a significant fraction of nonprompt background while WZ production is responsible for most of the backgrounds in the WZ VR. Distributions of leading lepton  $p_T$  and leading lepton  $\eta$  in WZ control region can be found in Figure 14.3. The nonprompt VRs are further discussed in chapter 15.

Selection criteria used to define different regions are illustrated in Figure 14.2 and is summarized in Table 14.1.

### 14.3 Kinematic Reconstruction

As mentioned, the LFV  $e\mu$  pair in assumed to be the product of the CLFV interaction, while the third lepton, referred to as the standalone lepton, is assumed to originate from the leptonically

Channel	Region	OnZ	OffZ	MET > 20 GeV	njet>=1	nbjet<=1
	VR	-	-	-	-	-
eee	WZ VR	$\checkmark$	-	$\checkmark$	$\checkmark$	$\checkmark$
	SR	-	✓	<b>√</b>	<b>√</b>	<b>√</b>
e $\mu\ell$	Nonprompt VR	$\checkmark$	-	-	-	-
	WZ VR	$\checkmark$	-	$\checkmark$	$\checkmark$	$\checkmark$
	Nonprompt VR	-	-	-	-	-
μμμ	WZ VR	-	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$

**Table 14.1:** Summary of the selection criteria used to define different event regions. "OnZ" means the presence of at least one OSSF pair with an invariant mass between 50 GeV and 106 GeV. Events are labelled as "OffZ" when they fail "OnZ" criteria.

decaying top quark. To distinguish this top quark ( $t \rightarrow \ell \nu b$ ) with the top quark that decays via the CLFV interaction ( $t \rightarrow e \mu q$ ), the former is referred to as the SM top quark while the latter is referred to as the LFV top quark.

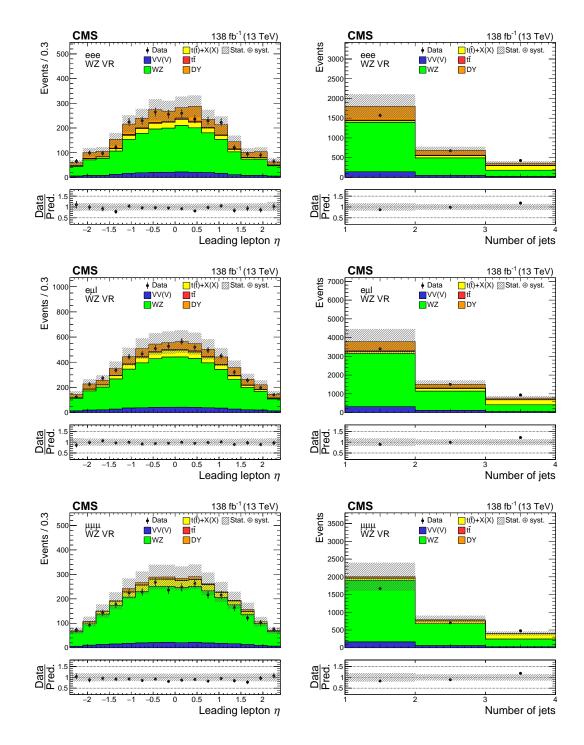
Jet with the highest b-tagging score, regardless of whether or not it crosses the medium working point threshold, is assumed to originate from bottom quark decay. Therefore, it is combined with MET and to build the SM top quark. The x and y component of MET are taken as measurements of neutrino  $p_x$  and  $p_y$ . The z component of neutrino momentum is calculated by imposing the constraint that the invariant mass of the combined object (standalone lepton + neutrino) must be equal to W boson mass. If there is no real solution, the real part of the complex solution is taken. If there is more than one real solution, the solution that is the closest to the  $p_z$  of the standalone lepton is taken. In events where there is more than one candidate of standalone lepton (i.e. the presence of the SSSF pair), the lepton that gives a top mass that is the closest to the the SM top quark mass ( $m_t = 172.5 \text{ GeV}$ ) is taken as the standalone lepton.

Once the standalone lepton has been determined, the remaining two leptons are labelled as the LFV e $\mu$  pair and is combined with each selected jet to reconstruct the LFV top quark candidates. Jet with the highest b-tagging score is excluded from this reconstruction since it is assumed to be from the decay of the SM top quark. Out of all the LFV top quark candidates, the candidate that gives a top mass that is the closest to the the SM top quark mass is taken. The LFV top quark mass is set to 0 in events where there are less than two jets.

Z boson candidate is reconstructed using the OSSF pair, which is not guaranteed to be present in the  $e\mu\ell$  channel. The Z boson mass (m<sub>Z</sub>) is set to 0 in events where the OSSF is absent. Z boson candidate is the only heavy particle reconstructed in the eee and  $\mu\mu\mu$  channels. Since

there are always two ways to form the OSSF pair, the OSSF pair with an invariant mass that is closer to the Z boson mass ( $m_Z = 91.2$  GeV) is taken.

Jets with high b-tagging scores are combined with leptons to form so called " $m_{b\ell}$ " systems. The first  $m_{b\ell}$  system takes the jet with the highest b-tagging score and combine it with each tight lepton in events. Out of the three  $m_{b\ell}$  system candidates, the one with the lowest  $m_{b\ell}$  is taken, the two constitutes are excluded from the consideration of the second  $m_{b\ell}$  system. If additional jets exist, the second  $m_{b\ell}$  system takes jet with the highest b-tagging score and combine it with two of the remaining leptons separately. Out of the two candidates, the one with lowest  $m_{b\ell}$  is taken.  $m_{b\ell}$  is set to 0 if no additional jet exists after the formation of the first  $m_{b\ell}$  system.



**Figure 14.3:** Distributions of the leading lepton  $\eta$  (left column) and the jet multiplicity (right column) in the WZ VRs. Events in the eee,  $e\mu\ell$ , and  $\mu\mu\mu$  WZ VRs are shown in the upper, middle, and lower row, respectively. The data are shown as filled points and the background predictions as histograms. All backgrounds are estimated with MC simulation. The hatched bands indicate statistical and systematic uncertainties for the background predictions. The last bin of the right column histograms includes the overflow events.

# Chapter 15

# **Nonprompt Background Estimation**

In this analysis, the term *prompt* leptons refers to leptons that originate from the CLFV vertex, the Drell-Yan process, or an electroweak boson decay, including leptons from  $\tau$  decays if the  $\tau$  lepton originates from the latter two processes. *Nonprompt* leptons refer to leptons that originate from hadron decays and photon conversions, as well as particles misidentified as leptons. *Nonprompt* leptons are suppressed through isolation requirements and a multivariate analysis (MVA)-based identification specifically trained to reject them.

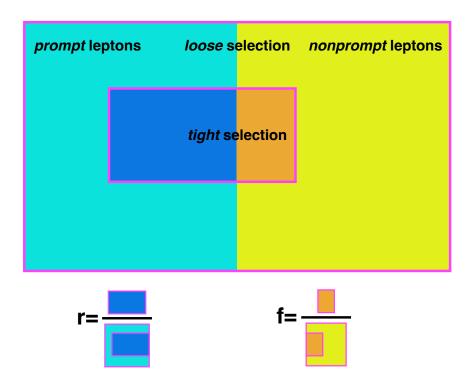
Nonprompt backgrounds are defined to be backgrounds with at least one nonprompt lepton passing the tight selection criteria, in this case generally dominated by Drell-Yan and  $t\bar{t}$  production. An accurate estimation of nonprompt backgrounds is difficult to achieve through MC modelling. Therefore, a data-driven technique called the "matrix method" [26] is used to estimate the nonprompt backgrounds.

A brief description of the *matrix method* in its simplist form is given in section 15.1 followed by its generalization and implementation in section 15.2. This method is validated using three VRs and is described in section 14.2. Lastly, the *nonprompt* estimation in the SR is presented in section 15.4.

#### 15.1 The Matrix Method

The *matrix method* is a data driven technique used to estimate the fraction of *nonprompt* leptons that pass a given lepton selection, referred to as "tight". The tight selection usually incorporates tight lepton identification and isolation requirements and corresponds to the full lepton selection used in an analysis. The *loose* selection is obtained by loosening the tight selection. The *loose* selection is used as a baseline such that any *loose* leptons fall into one of the two exclusive categories: tight or not tight. The matrix method deals with prompt and nonprompt leptons separately. As a result, prompt and nonprompt efficiencies are introduced, as is illustrated in Figure 15.1.

In a simplified scenario with only one lepton in the final state, the *prompt* efficiency r measures the probability of *prompt* leptons pass tight selection. It is treated as an observable that can be obtained through measurement,



**Figure 15.1:** Illustration of the *prompt* efficiency r and the *nonprompt* efficiency f.

$$r = \frac{n_P^T}{n_P^T + n_P^{\overline{T}}},\tag{15.1}$$

in which  $n_P^T/n_P^{\overline{T}}$  denotes the number of events with a *prompt* lepton that is *tight/not tight*. Similarly, *nonprompt* efficiency f can be expressed as,

$$f = \frac{n_N^T}{n_N^T + n_N^{\overline{T}}},\tag{15.2}$$

in which  $n_N^T/n_N^{\overline{T}}$  denotes the number of events with a *nonprompt* lepton that is  $tight/not\ tight$ .

The measurement of r/f is often performed in dedicated control regions, where high purity of prompt/nonprompt leptons is expected. These regions are referred to as the MR. It is assumed that r/f is a universal property of prompt/nonprompt leptons that is independent of physics processes. Therefore, r/f extracted from MR can be used to estimate the contamination of nonprompt leptons in a different region (e.g. SR) even though these two regions are orthogonal to each other.

In this simplified scenario, the total number of events in the region of interest (e.g. SR/VR) with a *tight*/not *tight* lepton can be expressed in a system of equations,

$$N^{T} = N_{P}^{T} + N_{N}^{T}$$

$$N^{\overline{T}} = N_{P}^{\overline{T}} + N_{N}^{\overline{T}},$$
(15.3)

in which capital letter "N" is used to indicate that these numbers are referring to events in a region that is different from MR.  $N_P^{\overline{T}}/N_N^{\overline{T}}$  can be expressed in terms of r/f and  $N_P^T/N_N^T$  according to Equation 15.1/15.2 and the assumption that r/f remains the same across different regions,

$$N^{T} = r \frac{N_{P}^{T}}{r} + f \frac{N_{N}^{T}}{f}$$

$$N^{\overline{T}} = (1 - r) \frac{N_{P}^{T}}{r} + (1 - f) \frac{N_{N}^{T}}{f}.$$

$$(15.4)$$

Equation 15.4 can also be expressed in the form of matrix,

$$\begin{pmatrix} N^T \\ N^{\overline{T}} \end{pmatrix} = \begin{pmatrix} r & f \\ 1 - r & 1 - f \end{pmatrix} \begin{pmatrix} N_P^T/r \\ N_N^T/f \end{pmatrix}.$$
(15.5)

Regions that correspond to the two numbers that appear in the righthand side vector of Equation 15.5 are referred to as the "application regions (ARs)", which can be constructed using experimental data. The estimation of *nonprompt* background, denoted by  $N_N^T$ , can be obtained by a simple matrix inversion.

## 15.2 Generialization and Implementation of the Matrix Method

The description in previous section deals with a scenario where only one lepton is studied. This analysis uses a generalized version of the *matrix method*, where all three *tight* leptons are considered to be possibly *nonprompt*. Equation 15.5 is generalized as,

$\left(N^{TTT}\right)$	r1r2r3	$n_1n_2f_3$	กรร	$r_1f_2f_3$	$f_1r_2r_3$	$f_1r_2f_3$	$f_1f_2r_3$	$f_1f_2f_3$	$N_{PPP}^{TTT}/r_1r_2$	r3)
$N^{TTT}$	$r_1r_2(1-r_3)$	$r_1 r_2 (1 - f_3)$	$r_1f_2(1-r_3)$	$r_1f_2(1-f_3)$	$f_1r_2(1-r_3)$	$f_1r_2(1-f_3)$	$f_1f_2(1-r_3)$	$f_1f_2(1-f_3)$	$N_{PPN}^{TTT}/r_1r_2$	f <sub>3</sub>
$N^{TTT}$	$r_1(1-r_2)r_3$	$r_1(1-r_2)f_3$	$r_1(1-f_2)r_3$	$r_1(1-f_2)f_3$	$f_1(1-r_2)r_3$	$f_1(1-r_2)f_3$	$f_1(1-f_2)r_3$	$f_1(1-f_2)f_3$	$N_{PNP}^{TTT}/r_1f_2$	- 1
$N^{T\overline{T}T}$	$r_1(1-r_2)(1-r_3)$	$r_1(1-r_2)(1-f_3)$	$r_1(1-f_2)(1-r_3)$	$r_1(1-f_2)(1-f_3)$	$f_1(1-r_2)(1-r_3)$	$f_1(1-r_2)(1-f_3)$	$f_1(1-f_2)(1-r_3)$	$f_1(1-f_2)(1-f_3)$	$N_{PNN}^{TTT}/r_1f_2$	f3
$N^{\overline{T}TT}$	$(1-r_1)r_2r_3$	$(1-r_1)r_2f_3$	$(1-r_1)f_2r_3$	$(1-r_1)f_2f_3$	$(1-f_1)r_2r_3$	$(1-f_1)r_2f_3$	$(1-f_1)f_2r_3$	$(1-f_1)f_2f_3$	$N_{NPP}^{TTT}/f_1r_2$	r3
$N^{\overline{T}T\overline{T}}$	$(1-r_1)r_2(1-r_3)$	$(1-r_1)r_2(1-f_3)$	$(1-r_1)f_2(1-r_3)$	$(1-r_1)f_2(1-f_30$	$(1-f_1)r_2(1-r_3)$	$(1-f_1)r_2(1-f_3)$	$(1-f_1)f_2(1-r_3)$	$(1-f_1)f_2(1-f_3)$	$N_{NPN}^{TTT}/f_1r_2$	f3
$N^{\overline{T}\overline{T}T}$	$(1-r_1)(1-r_2)r_3$	$(1-r_1)(1-r_2)f_3$	$(1-r_1)(1-f_2)r_3$	$(1-r_1)(1-f_2)f_3$	$(1-f_1)(1-r_2)r_3$	$(1-f_1)(1-r_2)f_3$	$(1-f_1)(1-f_2)r_3$	$(1-f_1)(1-f_2)f_3$	$N_{NNP}^{TTT}/f_1f_2$	3
$\left(N^{\overline{\tau}\overline{\tau}\overline{\tau}}\right)$	$(1-r_1)(1-r_2)(1-r_3)$	$(1-r_1)(1-r_2)(1-f_3)$	$(1-r_1)(1-f_2)(1-r_3)$	$(1-r_1)(1-f_2)(1-f_3)$	$(1-f_1)(1-r_2)(1-r_3)$	$(1-f_1)(1-r_2)(1-f_3)$	$(1-f_1)(1-f_2)(1-r_3)$	$(1-f_1)(1-f_2)(1-f_3)$ (15.6)	$\int \left( N_{NNN}^{TTT}/f_1f_2 \right)$	§)

All but the first number that appear in the righthand side vector correspond to events with at least one *nonprompt* lepton that pass *tight* selection criteria. Therefore, the overall *nonprompt* background is expresses as,

$$N_{Nonprompt}^{TTT} = N_{PPN}^{TTT} + N_{PNP}^{TTT} + N_{PNN}^{TTT} + N_{NPP}^{TTT} + N_{NNP}^{TTT} + N_{NNP}^{TTT} + N_{NNN}^{TTT},$$
(15.7)

which can be obtained by first constructing 8 ARs to form the lefthand side vector. Secondly, the  $8 \times 8$  matrix is constructed and inverted. Lastly, the righthand side vector can be obtained by multiplying the lefthand side vector to the inverted matrix.

Only two PDs "SingleElectron" and "SingleMuon" are used in the construction of MR in 2016 and 2017 while "SingleElectron" is replaced with "EGamma" in 2018. In addition to PDs, the measurements of r/f also utilize the  $t\bar{t}$  sample and all MC samples listed under the "prompt background" category in Table 12.3. Depending on the flavor of the leading lepton in MC, events are selected with either a single-electron or a single-muon trigger, which is summarized in Table 15.1. Data events are selected with the same HLT triggers as well but events in "SingleMuon" ("SingleElectron" or "EGamma") PD are only accepted if the leading lepton is a muon (electron).

Channel	Path	Dataset	2016	2017	2018
Electron	HLT_Ele27_WPTight_Gsf	Data & MC	$\checkmark$	-	-
Electron	HLT_Ele35_WPTight_Gsf	Data & MC	-	$\checkmark$	$\checkmark$
Muon	HLT_IsoMu27	Data & MC	$\checkmark$	$\checkmark$	$\checkmark$

**Table 15.1:** Summary of the HLT triggers used in the measurement of r and f.

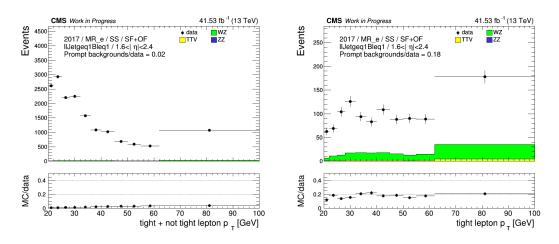
Both r and f are parameterized in bins of lepton  $p_T$ ,  $|\eta|$ , and jet multiplicity. The bin range is optimized to retain sufficient statistics for each bin:

- Electron p<sub>T</sub> bin range: {20.0, 24.6, 28.8, 33.0, 37.2, 41.4, 46.1, 52.1, 59.3, 68.3, 82.7, 110.6} GeV,
- Muon p<sub>T</sub> bin range: {20.0, 23.8, 27.7, 31.3, 35.0, 38.9, 42.8, 45.6, 50.7, 59.5, 72.9, 94.3}
   GeV,
- $|\eta|$  bin range: {0, 0.8, 1.6, 2.4},
- Jet multiplicity:  $\{0 \text{ jet}, \geq 1 \text{ jet}\}.$

The jet multiplicity bin is a proxy for variation of the composition of physics processes. In addition to requiring at least one jet, the MR corresponds to the second jet multiplicity bin requires no more than one b-tagged jet as this is also required in the SR.

The *nonprompt* efficiency is measured in same-sign dilepton regions, in which the leading lepton in  $p_T$ , used as a tag, is required to be matched with trigger objects within  $\Delta R < 0.2$ . The sub-leading lepton is required to pass the *loose* selection and is taken as the *probe*. Events that have two same-sign electrons with an invariant mass between 76 GeV and 106 GeV are removed from MR to suppress the backgrounds that originate from charge misidentification. No such requirement has been introduced to the muon MR due to its negligible rate of charge misidentification.

The contribution from *prompt* backgrounds, estimated from MC simulation, are subtracted from data. A representative composition of backgrounds in MR is shown in Figure 15.2.



**Figure 15.2:** Distribution of lepton  $p_T$  in a representative electron *nonprompt* efficiency MR. In this particular example, both ee and  $\mu$ e flavor composites are considered. At least one jet and at most one b-tagged jet are required (the second jet multiplicity bin). *Probe* electron is required to have  $1.6 < |\eta| < 2.4$  (the third  $\eta$  bin). Contamination from *prompt* backgrounds are estimated with MC simulation, and are shown as histograms. The data are shown as filled points. From left to right: *loose* (i.e. *tight* + *not tight*) electron  $p_T$ , *tight* electron  $p_T$ .

The fake efficiency f is calculated as:

$$f = \frac{n_{data}^{tag+tight} - n_{MC(prompt)}^{tag+tight}}{n_{data}^{tag+loose} - n_{MC(prompt)}^{tag+loose}},$$
(15.8)

where the numerator is selected with one *tag* and one *tight* lepton while the denominator is selected with one *tag* and one *loose* lepton. The selection criteria for *tag*, *loose*, and *tight* lepton is summarised in Table 15.3.

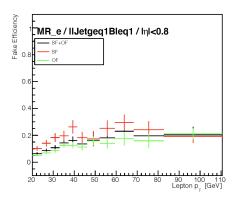
Lepton	Selection	loose	tag	tight <sup>ii</sup>	
	PΤ	> 20 GeV	$>$ 38 $\mathrm{GeV}^{\mathrm{i}}$	> 20 GeV	
Electron	/rel mini	< 0.4	< 0.1	< 0.12	
Liection	TOP LEPTONMVA	>-0.9	>0.95	>0.9	
	Match with trigger objects	-	$\checkmark$	-	
	Рт	> 20 GeV	> 30 GeV	> 20 GeV	
	/rel mini	< 0.4	< 0.1	< 0.12	
Muon	Cut-based ID	-	Medium WP	Medium WP	
	TOP LEPTONMVA	>0.5	>0.9	>0.9	
	Match with trigger objects	-	$\checkmark$	-	

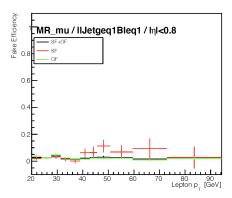
**Table 15.2:** Summary of the lepton selections needed for the measurement of r and f. Please note: (i) the minimum  $p_T$  cut for tag electron in 2016 dataset is reduced to 30 GeV to adjust for the trigger threshold, and (ii) the tight selection here is the same as the tight lepton selection described in section 13.1.

The measured *nonprompt* efficiency f exhibits a dependency on flavor composition, as is shown in Figure 15.3. This dependency is treated as a source of the systematic uncertainties of the *nonprompt* estimation and is further discussed in section 17.2.

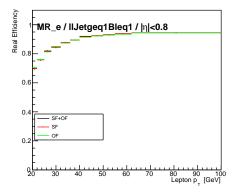
The prompt efficiency r is measured in simulated  $t\bar{t}$  events in opposite-sign dilepton regions. The same lepton selection listed in Table 15.2 is used to perform the Tag-and-Probe. The leading lepton in  $p_T$  is used as a tag while the oppositely charged sub-leading lepton is taken as a probe. The variation of r between different flavor composition is negligible, as is shown in Figure 15.4. Therefore, only  $e\mu$  events are used to measure prompt efficiency in order to minimise the contamination of prompt leptons.

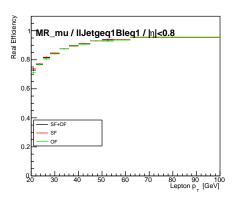
The selection criteria for various MRs is summarised in Table 15.3.





**Figure 15.3:** Representative *nonprompt* electron efficiency measured in data events. From left to right: electron f, muon f. Events with a same-flavor lepton pair are shown in red points while events selected with a different-flavor lepton pair are shown in green points. Events with a same-flavor or different-flavor lepton pair is shown in black points. These plots correspond to the first  $|\eta|$  bin ( $|\eta| < 0.8$ ) and the second jet multiplicity bin. Events selected Error bars displayed in these plots include statistical uncertainty only.





**Figure 15.4:** Representative *prompt* efficiency measured in simulated  $t\bar{t}$  events. From left to right: electron r, muon r. Events with a same-flavor lepton pair are shown in red points while events selected with a different-flavor lepton pair are shown in green points. Events with a same-flavor or different-flavor lepton pair is shown in black points. These plots correspond to the first  $|\eta|$  bin  $(|\eta| < 0.8)$  and the second jet multiplicity bin. Error bars displayed in these plots include statistical uncertainty only.

#### 15.3 Validation of the Matrix Method

The performance of the *matrix method* is validated using three regions that are tangential to the SR, referred to as VRs. In these VRs, *prompt* backgrounds are estimated using MC simulation while *nonprompt* background is estimated with the *matrix method*. A summary of the selections

Observable	jet bin	# of selected leptons	lepton flavor composite	$ \sum_i C_i $	OffZ	njet	nbjet
f	0 jet	2	any	2	same-sign ee	= 0	= 0
,	1 or more jet	2	any	2	same-sign ee	≥ 1	$\leq 1$
r	0 jet	2	eμ only	0	-	= 0	= 0
,	1 or more jet	2	eμ only	0	-	$\geq 1$	$\leq 1$

**Table 15.3:** Summary of the cuts applied to the r/f measurement region.

applied to these VRs is given in chapter 14.

Distribution of the leading lepton  $\eta$  and jet multiplicity are shown in Figure 15.5. Good agreement between data and background estimate has been observed in all three VRs.

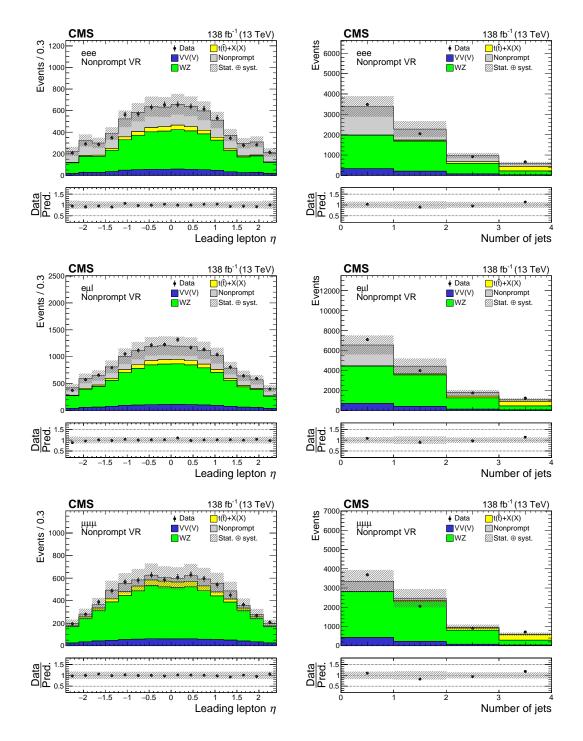
### 15.4 Nonprompt Estimate in SR

The *matrix method* is used to estimate *nonprompt* background in the SR. Distributions of the LFV e $\mu$  mass and the Z boson mass are shown in Figure 15.6. When compared to background estimate from pure MC simulation (Figure 14.1), the updated background template is smoother with lower statistical uncertainties.

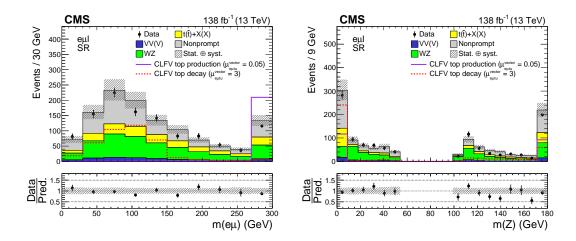
The number of expected events from various kinds of backgrounds are shown in Table 15.4.

**Table 15.4:** Expected background contributions and the number of events observed in data collected during 2016–2018. The statistical and systematic uncertainties are added in quadrature. The category "other backgrounds" includes smaller background contributions containing one or two top quarks plus a boson or quark. The CLFV signal, generated with  $C_{\rm eutu}^{\rm vector}/\Lambda^2=1{\rm TeV}^{-2}$ , is also listed for reference. The signal yields include contributions from both top production and decay modes.

Process	m(eμ)<150 GeV	m(eμ)>150 GeV	
Nonprompt	$351 \pm 92$	$146\pm38$	
WZ	$275 \pm 64$	$145\pm35$	
ZZ	$33.2 \pm 6.5$	$13.1 \pm 2.6$	
VVV	$17.0 \pm 8.5$	$12.0 \pm 6.0$	
$t \bar{t} W$	$47.6 \pm 10.0$	$40.0 \pm 9.1$	
tīZ	$39.1 \pm 7.9$	$25.8 \pm 5.4$	
tŧH	$28.2 \pm 4.5$	$10.0 \pm 1.6 \\ 2.5 \pm 0.5$	
tZq	$5.5\pm1.1$		
Other	$7.3\pm 3.7$	$4.5\pm 2.3$	
Total expected	$805\pm123$	$398 \pm 57$	
Data	783	378	
CLFV	$207\pm15$	$4440\pm215$	



**Figure 15.5:** Distributions of the leading lepton  $\eta$  (left column) and the jet multiplicity (right column) in the *nonprompt* VRs. Events in the eee, eμ $\ell$ , and μμμ *nonprompt* VRs are shown in the upper, middle, and lower row, respectively. The data are shown as filled points and the SM background predictions as histograms. The *nonprompt* background is estimated using control samples in data, while other backgrounds are estimated using MC simulation. The hatched bands indicate statistical and systematic uncertainties for the SM background predictions. The last bin of the right histogram includes the overflow events.



**Figure 15.6:** Distributions of the LFV e $\mu$  mass (left) and the Z boson mass (right) in SR. The data are shown as filled points and the SM background predictions as histograms. The *nonprompt* background is estimated using control samples in data, while other backgrounds are estimated using MC simulation. The hatched bands indicate statistical and systematic uncertainties for the SM background predictions. The normalisation of the signal processes is chosen arbitrarily for improved visualisation. The last bin of both histograms includes the overflow events.

# Chapter 16

# Signal Extraction with Boosted Decision Trees

A MVA is performed in SR to further separate the LFV signals from the backgrounds, and enhance the sensitivity of this analysis. More specifically, a dozen of discriminating variables, referred to as "features", are selected and combined by a gradient-BDT, which is implemented using the XGBOOST package [27]. There are several reasons why BDT is chosen: (i) the goal of the MVA is to achieve maximum separation between signals and backgrounds using a small number of already well-separated kinematic variables, instead of exploring some complicated structures hidden in event topology, (ii) under such a goal, the potential performance gain from a more sophisticated algorithm like a NN is limited, (iii) a BDT-based algorithm is straightforward to implement and consumes only a moderate amount of computational resources, and (iv) the interpretability of a BDT-based algorithm is excellent.

The top production and decay signals are longer distinguished by the BDT. They are combined into a single signal class, just like all backgrounds are combined into a single background class. The training of the BDT depends entirely on MC samples that are statistically orthogonal to the samples used in the actual background estimation. More details on the configurations of the BDT are described in section 16.1. The input features are described in section 16.2. The output of the BDT is presented in section 16.3.

## 16.1 BDT Configuration

The LFV e $\mu$  mass of the top decay signal is bounded by the SM top quark mass, as is shown in Figure 14.1. On the contrary, the LFV e $\mu$  mass of the top production signal has no such restriction and often reaches TeV level. Therefore, a 150 GeV threshold is used to divide the SR into two SRs enriched in different signal modes. The MVA strategy is to combine two signal modes within each SR and train binary BDTs separately for each SR. In other words, only two signal datasets and two background datasets are needed.

Other aspects of the signal MC samples, such as the Lorentz structure and the flavor of the up-type quark involved in LFV interaction, are shown to have a relatively small impact on the kinematics of final state particles, as is shown in Figure 16.1. Therefore, they are not distinguished by the BDT. The construction of the signal datasets take a few steps. Firstly, all top production

signal samples, regardless of the Lorentz structure or the quark flavor, are normalised to the cross section of the vector-like operator with an e $\mu$ tu vertex, which is shown in Figure 12.2. Similarly, all top decay signals samples are normalised to the cross section of the vector-like operator. For each sample, a normalisation weight is calculated and is absorbed by the MC weight, which originally only covers per-event correction. These updated weights are eventually passed on to the BDT to weight each signal event. Secondly, all top production and decay signal samples are combined into a single dataset, which is then divided into two subsets using a 150 GeV threshold on LFV e $\mu$ .

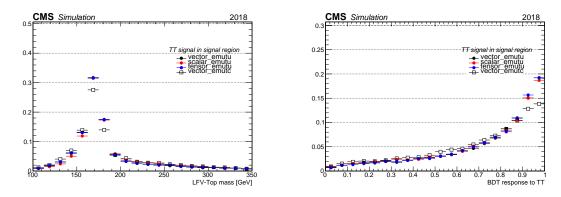
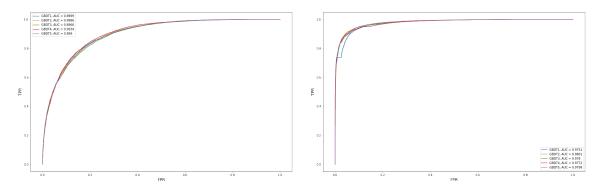


Figure 16.1: Normalized distribution in SR1. From left to right: LFV top mass, BDT shape

All background MC samples listed in Table 12.3 are used in the BDT training. The



**Figure 16.2:** ROC curve with 5-fold cross validation. From left to right: BDT targeting TT (SR1), BDT targeting ST (SR2).

The MC dataset is divided into 5 subsets evenly. A 5-fold cross-validation scheme is deployed: the training set consists of 3 out of the 5 subsets, while validation/testing set each consists of 1 subset. The number of estimators is set to 1000, max depth 5, and sub-sample 0.8 with the evaluation metric set to "mlogloss". The results of the cross-validation study are shown in Figure 16.2. The trained BDT model targeting TT(ST) signal is used to evaluate each event in SR1(SR2): a BDT weight is assigned to each event, giving the likelihood that it originated from TT(ST) signal.

#### 16.2 BDT Features

The observables used in training are referred to as "features" in this analysis. The following features are used for both ST and TT classifier:

- MVA  $M_{e\mu}$ : invariant mass of the Opposite-Sign  $e\mu$  pair
- MVA LFVePt:  $p_T$  of the flavor-violating electron
- MVA LFVmuPt:  $p_T$  of the flavor-violating muon
- MVA LFVTopmass: invariant mass of the flavor-violating top-quark candidate
- MVA Zmass: invariant mass of Z boson candidate
- MVA\_Jet2Btag: b-tagging score of the jet with the second highest b-tagging score
- MVA Mbl2: invariant mass of the second b-jet+lepton system
- MVA njet: number of jets
- MVA nbjet: number of b-jets
- MVA\_tM: transverse mass of the W boson candidate (from standard model top-quark)
- MVA IIDr:  $\Delta R$  between flavor-violating electron and muon
- MVA SSee Zmass: invariant mass of a Same-Sign di-electron pair
- MVA Topmass: invariant mass of the standard model top-quark candidate
- MVA Met: missing transverse energy

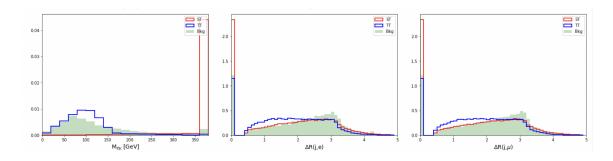
The following features are only used for TT classifier:

- MVA Ht: scalar sum of the  $p_T$  of all objects
- MVA Mbl1: invariant mass of the second bjet+lepton system
- MVA JeDr:  $\Delta R$  between flavor-violating electron and a light jet (non-b-jet)
- MVA JmuDr:  $\Delta R$  between flavor-violating muon and a light jet (non-b-jet)

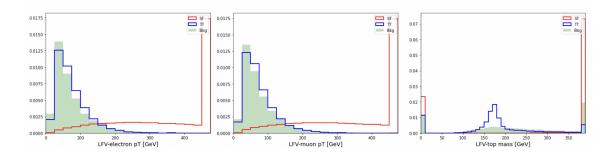
The following features are used for ST classifier:

- MVA BaPt:  $p_T$  of the standard model lepton
- MVA JetHt: scalar sum of the  $p_T$  of jets

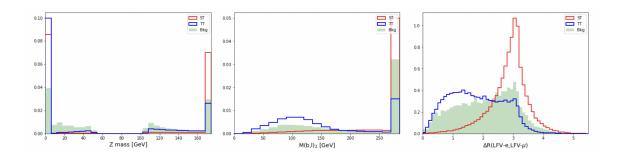
Distributions of selected features are shown in Figure 16.3-16.7.



**Figure 16.3:** Normalized distribution of various features in SR. From to left to right: MVA $\_M_{e\mu}$ , MVA JeDr, MVA JeDr.

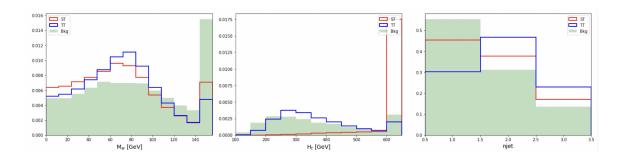


**Figure 16.4:** Normalized distribution of additional features in SR. From to left to right: MVA LFVePt, MVA LFVmuPt, MVA LFVTopmass.

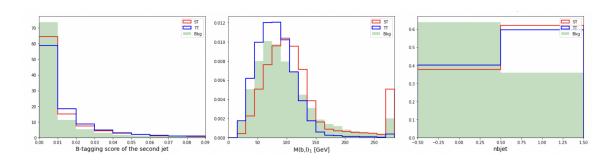


**Figure 16.5:** Normalized distribution of additional features in SR. From to left to right:  $MVA\_Zmass$ ,  $MVA\_Mbl2$ ,  $MVA\_IIDr$ .

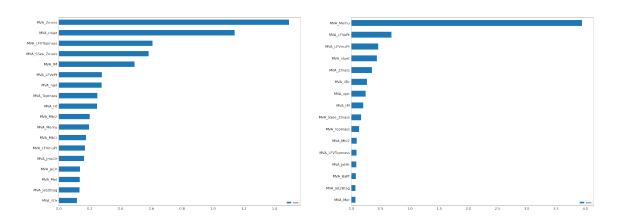
To determine the relative importance of these features, feature importance is extracted using the "gain" method and is shown in Figure 16.10.



**Figure 16.6:** Normalized distribution of additional features in SR. From to left to right: MVA\_tM, MVA Ht, MVA njet.



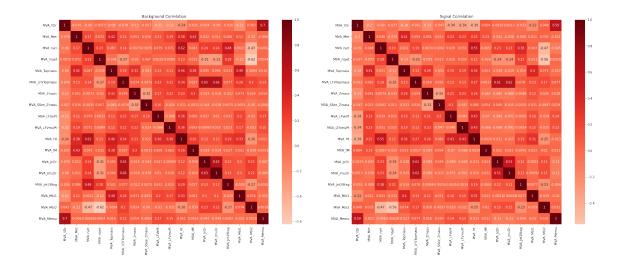
**Figure 16.7:** Normalized distribution of additional features in SR. From to left to right: MVA Jet2Btag, MVA Mbl1, MVA nbjet.



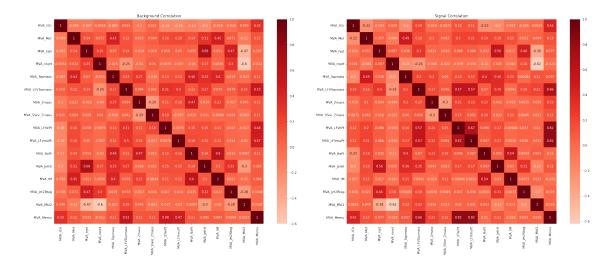
**Figure 16.8:** List of features ranked by their relative importance. From left to right: BDT targeting TT (SR1), BDT targeting ST (SR2)

## 16.3 BDT Output

The output of the BDTs are shown in Figure 16.11. Note: all but the nonprompt backgrounds are estimated with MC simulation. The nonprompt background backgrounds are estimated with

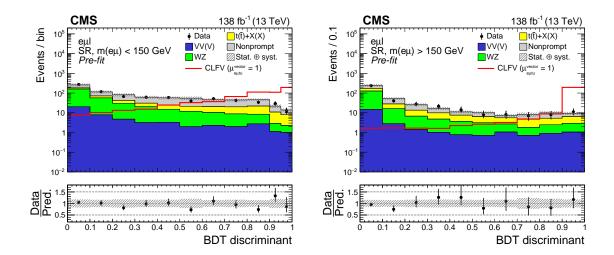


**Figure 16.9:** Correlation matrices (SR1), from left to right: background correlation, signal correlation.

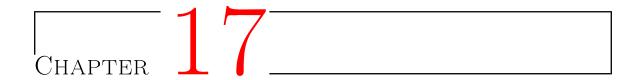


**Figure 16.10:** Correlation matrices (SR2), from left to right: background correlation, signal correlation.

the matrix method.



**Figure 16.11:** Distribution of BDT output, from left to right TT enriched SR (SR1), ST enriched SR (SR2)



# **Systematic Uncertainties**

For this analysis, we consider the following sources of systematic uncertainties:

### 17.1 Theoretical Uncertainties

- Prompt background cross-sections: These uncertainties arise from the uncertainties in the
  measured cross-sections of the processes which are used for scaling the MC to the luminosity
  of data. Systematic uncertainties associated to the prompt backgrounds WZ ( as discussed
  in autorefsec:CRWZ ), ZZ , ttW/ttZ/ttH, tZq are 6%, 6%, 15% and 20% respectively.
  Measurements performed on the WZ and ZZ processes currently have uncertainties of
  order 5-8% citeWZ2019 citeZZ2020. A 50 % normalization uncertainty is assigned to other
  smaller backgrounds.
- PDF: Using 100 the replicas of the NNPDF 3.1 set, the PDF uncertainties are obtained by taking the root mean square value of the variations. Only shape components of the variation is considered, this is done by normalizing LHE weights of the replicas such that the sum of the LHE wights (in SR) stays the same for each replica. This uncertainty treated as correlated. We consider this uncertainty for all the signals and major prompt backgrounds (i.e. WZ, TTZ, TTW and TTH).
- Renormalization and factorization scale: this uncertainty is evaluated by considering an envelope of 6 variation ( $\mu_R$  2,  $\mu_R$  0.5,  $\mu_F$  2,  $\mu_F$  0.5,  $\mu_R$  and  $\mu_F$  2,  $\mu_R$  and  $\mu_F$  0.5). This uncertainty is treated as correlated and only shape component is considered. We consider this uncertainty for all the signals and major prompt backgrounds (i.e. WZ, TTZ, TTW and TTH).
- ISR and FSR: initial state radiation and final state radiation uncertainty is evaluated by using the default set of variation (2 and 0.5). This uncertainty is treated as correlated and only shape component is considered. We consider this uncertainty for all the signals.

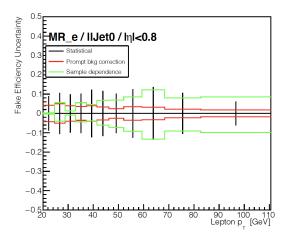
### 17.2 Nonprompt Uncertainties

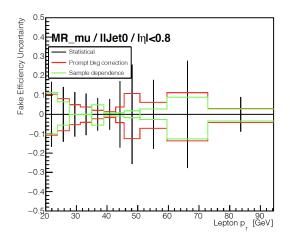
We consider the following sources of systematic uncertainties (shape) associated with the *fake* efficiency.

- Prompt background correction
- Sample dependence
- Statistical uncertainty

An important systematic uncertainty comes from the estimate of prompt contamination in MR. As is discussed in chapter 15, prompt backgrounds (estimated with MC) are subtracted from total event yields measured in MR (data). A flat 20 % uncertainty ( $\alpha$  in Equation 17.1) is assigned to the event yields of the prompt background and the resulting variation of f is taken as the uncertainty, which is estimated to be between 5 % and 15 %.

$$f = \frac{n_{data}^{T} - (1 + \alpha) n_{Prompt \ MC}^{T}}{n_{data}^{T + \overline{T}} - (1 + \alpha) n_{Prompt \ MC}^{T + \overline{T}}}.$$
(17.1)





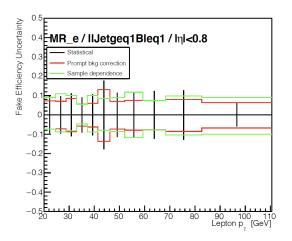
**Figure 17.1:** Comparison of different components of the uncertainties associated to the *fake* efficiency measured in 2017 dataset (njet=0 bin,  $|\eta| < 0.8$  bin). From left to right: electron f uncertainty, muon f uncertainty. Note: black uncertainty bars represent statistical uncertainties.

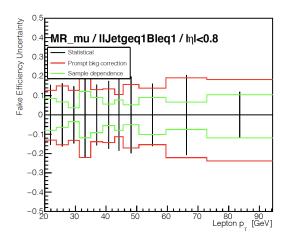
Sample dependence is one of the primary sources of systematic uncertainty and it is concerned with the possibility that the *fake* efficiency f measured in MR may not reflect characteristics of the non-prompt leptons in SR due to different compositions of backgrounds. This type of uncertainty is estimated by introducing a variation factor  $\beta$  between the proportions of Same-Flavor and Opposite-Flavor pairs in MR. For example, electron f can be calculated as (prompt background correction is ignored from the equation):

$$f_{e} = \frac{(1+\beta)n_{F,e+e}^{T} + (1-\beta)n_{F,e+\mu}^{T}}{(1+\beta)n_{F,e+e}^{T+\overline{T}} + (1-\beta)n_{F,e+\mu}^{T+\overline{T}}}.$$
(17.2)

A 20% variation ( $\beta$ ) is assigned the resulting variation of f is taken as the uncertainty, which is estimated to be between 3 % and 15 %.

A comparison of different sources of systematic uncertainties (using 2017 datasets) are shown in Figure 17.1 and Figure 17.2. A complete summary of uncertainties associated to *real* and *fake* efficiency can be found in.



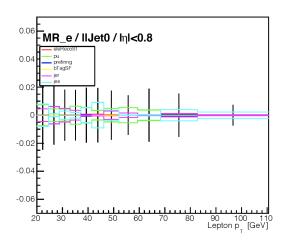


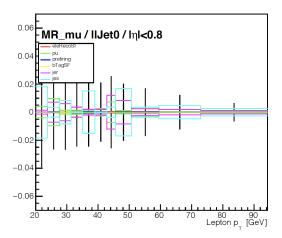
**Figure 17.2:** Comparison of different components of the uncertainties associated to the *fake* efficiency measured in 2017 dataset (njet>0 bin,  $|\eta|$  <0.8 bin). From left to right: electron f uncertainty, muon f uncertainty. Note: black uncertainty bars represent statistical uncertainties.

In addition to statistical uncertainties, MC uncertainties are propagated to the *real* efficiency as sources of systematic uncertainties:

- Statistical uncertainty
- MC uncertainty
  - Electron reconstruction
  - b-tagging
  - JES/JER
  - Pile-up rewighting
  - ECAL prefiring

The uncertainties associated to the *real* efficiency are relatively small when compared to the *fake* efficiency uncertainties. A comparison of different sources of *real* efficiency uncertainties are shown in Figure 17.3.





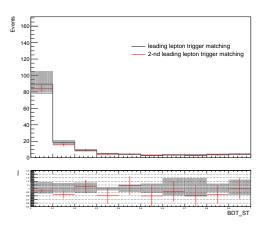
**Figure 17.3:** Comparison of different components of the uncertainties associated to the *real* efficiency measured in 2017 dataset (njet=0 bin,  $|\eta| < 0.8$  bin). From left to right: electron r uncertainty, muon r uncertainty. Note: black uncertainty bars represent statistical uncertainties.

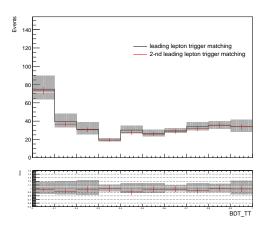
In addition to the four components (i.e.  $r_e$ ,  $r_\mu$ ,  $f_e$ ,  $f_\mu$ ) of the shape uncertainties associated to the measurement of r and f, a fifth component is considered that accounts for the potential bias introduced when implementing 3D matrix method: Four out of the eight regions that appear on the lefthand side of the Equation 15.6 (i.e.  $N^{\overline{T}TT}$ ,  $N^{\overline{T}TT}$ ,  $N^{\overline{T}TT}$ ,  $N^{\overline{T}TT}$ ) are selected by requiring the leading lepton to fail the *tight* criteria (See Table 15.2). Effectively this means that the isolation requirement is reversed for leading lepton that enter these four regions. Selecting the leading lepton by a loose/reversed isolation requirement is not ideal since the leading lepton is required to match with iso-trigger. To account for this bias, a 50 % uncertainty is assigned to the  $f_1$  (fake efficiency of the leading lepton) for events that enter these four regions. The variation of the non-prompt estimate due to trigger matching is largely covered by this uncertainty (See Figure 17.4).

The five components of the uncertainties discussed in this section are propagated through the matrix inversion. The resulting variations of the non-prompt estimates are taken as the shape uncertainties assigned to non-prompt backgrounds. These uncertainties are treated as correlated between the years. In addition to these shape uncertainties, an overall normalization uncertainty of 10% is assigned in order to cover any other potential bias.

### 17.3 Diboson Uncertainties

Mismodeling of the jet multiplicity is observed in WZ control region (See autorefsec:CRWZ). This is largely due to the fact that jets generated from diboson samples are coming from radiation (due to our trilepton selection). Therefore, the accuracy of the jet multiplicity distribution is suboptimal. To take this into account, a dedicated jet-dependent uncertainty is assigned to each





**Figure 17.4:** The impact of matching leptons to trigger objects on non-prompt estimate. From left to right: non-prompt estimate in ST enriched SR, non-prompt estimate in TT enriched SR. The nominal configuration of the matrix method is to match the leading lepton with trigger objects. Matching the 2nd-leading with the trigger objects is taken as an alternative to evaluate the robustness of the non-prompt estimate. The uncertainty band only covers the variation of the non-prompt estimate as a result of varying leading lepton f by 50 %. Uncertainty bars only include statistical uncertainties.

event. This uncertainty is determined using diboson control region:

- Exactly three leptons (any flavor composite),
- OnZ,
- MET>85GeV,
- Veto events with at least one b-tag jet ( $p_T > 20$ GeV).

The jet multiplicity distributions are shown in Figure 17.5. For each year, a scale factor parameterized as bins of jet multiplicity is derived:

$$\epsilon = \frac{N_{data} - N_{VVV} - N_{TX} - N_{TTbar} - N_{others}}{N_{VV}}.$$
 (17.3)

The scale factor  $\epsilon$  is used to estimate the uncertainty, denoted by  $\Delta$ :

$$\Delta = |1 - \epsilon| \tag{17.4}$$

This uncertainty is about 10-20%, as is shown in Figure 17.6.

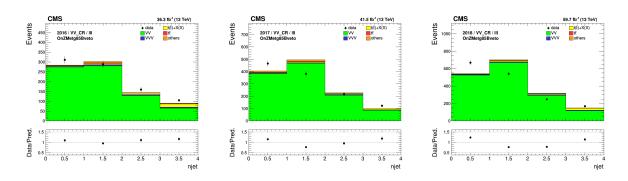
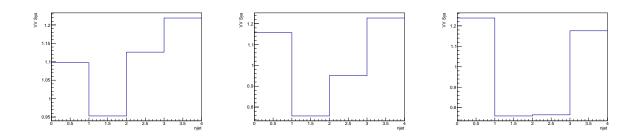


Figure 17.5: Diboson control region, from left to right: 2016, 2017 and 2018 datasets.



**Figure 17.6:** Scale factors derived from diboson control region, from left to right: 2016, 2017 and 2018 datasets.

## 17.4 Other Experimental Uncertainties

- Lepton reconstruction, identification, and isolation: electron/muon reconstruction uncertainties are provided by relevant POG. Uncertainties associated with lepton identification and isolation scale factors were evaluated by the authors of the mvaTOP ID citemvaTOP. The statistical components of these uncertainties are treated as uncorrelated while the other components are treated as fully correlated. For high  $p_T$  muons ( $p_T > 200 \text{GeV}$ ), an additional uncertainty (denoted "mulDHighPt") is assigned and it increases linearly from 0 to 10% (200 GeV-1000 GeV) and is caped at 10% after 1000 GeV.
- Muon scale uncertainties: uncertainties on muon momentum (denoted "MuonScale") are assigned using different method according to the muon  $p_T$ : Rochester algorithm is used for low  $p_T$  muons ( $p_T$  <200Gev), while GEciteGEmethod method is used for high  $p_T$  muons ( $p_T$  >200Gev).
- b-tagging: b-tagging efficiency and uncertainty is provided by the BTV group.
- trigger scale factor: trigger scale factors are set to 1 and a flat 2% uncertainty is assigned. This uncertainty is treated as uncorrelated.

- Luminosity: The uncertainties of 1.0%, 2.0% and 1.5% are assigned to the integrated luminosity for 2016, 2017, 2018, respectively. When processing the run 2 data the individual year uncertainties are treated as uncorrelated while there are two additional correlated luminosity uncertainties; firstly, 0.6%, 0.9% and 2.0% for each year respectively to account for the correlation between 2016, 2017 and 2018 data and secondly, 0.6%, 0.2% for 2017 and 2018 respectively to account for the correlation between 2017 and 2018 data.
- jet energy scale and resolution: The jet energy scale, JES, and jet energy resolution, JER, are centrally provided by the JET/MET POG citeJEC. Variations of jet energy scale and resolution are propagated to the MET and b-tagging SF.
- pile-up reweighting: The measured minimum bias cross-section is varied up and down by 4.6%. This uncertainty is treated as correlated.
- MET unclustered missing energy is considered and treated as uncorrelated across the years.
- L1 ECAL prefiring: In the 2016 and 2017 datasets, L1 EGamma triggers fired early causing
  many uninteresting events to be recorded while the later interesting events were rejected.
  Since this effect is not present in the MC simulation, a tool citeECALPre provided by the
  L1 DPG is used to reweight MC events. This uncertainty is treated as correlated.
- HEM15/16 Issue: The HEM15/16 issue refers to two HCAL modules whose power supply died in the middle of the data taking (runs>=319077, i.e. last certified run of 2018B, and all of 2018C+D). The HEM issue is likely a very small effect but we still have to check it following the procedure in citeHEM

Uncertainties related to B-tagging scale factors are split into different sources. For b and udsg jets, we applied If, hf, hfstats1/2, and lfstats1/2 uncertainties. For c jets, we applied cferr1/2 uncertainties. Correlations between different sources are specified in the Table 17.1.

**Table 17.1:** A hyphen (-) denotes that a source is not correlated between the different years.

Source	Correlated	Description
lf	✓	udsg+c jets in heavy flavor region
hf	$\checkmark$	b+c jets in light flavor region
hfstats1	-	Linear fluctuations of c jets
hfstats2	-	Quadratic fluctuations of c jets
lfstats1	-	Linear fluctuations of udsg jets
lfstats2	-	Quadratic fluctuations of udsg jets
cferr1	$\checkmark$	Linear fluctuations of c jets
cferr2	$\checkmark$	Quadratic fluctuations of c jets

### 17.4.1 Jet energy scale uncertainties

Uncertainties associated with JES are split into their 27 components and properly treated the correlations of the split uncertainties by year as recommended by the JETMET POG and described in the Table 17.2.

**Table 17.2:** Summary of the sources of uncertainty related to the JECs. A hyphen (-) denotes that a source is not correlated between the different years.

Source	Correlated	Source	Correlated
AbsoluteStat	-	RelativePtHF	✓
AbsoluteScale	$\checkmark$	RelativeBal	$\checkmark$
${\sf Absolute MPFB} ias$	$\checkmark$	RelativeSample	-
Fragmentation	$\checkmark$	RelativeFSR	-
SinglePionECAL	$\checkmark$	RelativeStatFSR	$\checkmark$
${\sf Single Pion HCAL}$	$\checkmark$	RelativeStatEC	-
${\sf FlavorQCD}$	$\checkmark$	RelativeStatHF	-
TimePtEta	-	PileUpDataMC	$\checkmark$
RelativeJEREC1	-	PileUpPtRef	$\checkmark$
RelativeJEREC2	-	PileUpPtBB	$\checkmark$
RelativeJERHF	$\checkmark$	PileUpPtEC1	$\checkmark$
RelativePtBB	$\checkmark$	PileUpPtEC2	$\checkmark$
RelativePtEC1	-	PileUpPtHF	$\checkmark$
RelativePtEC2	-		

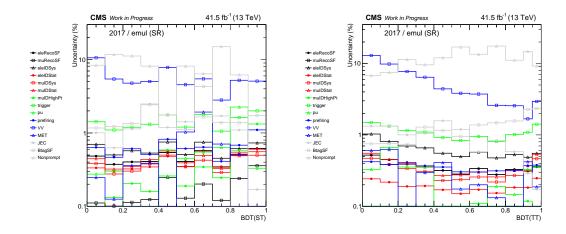
B-tagging scale factors and MET vector are computed for each of the JES templates and treated as uncertainties that are fully correlated to the respective JES sources.

The overall systematic uncertainty on background is estimated to be about 15 % in SR.

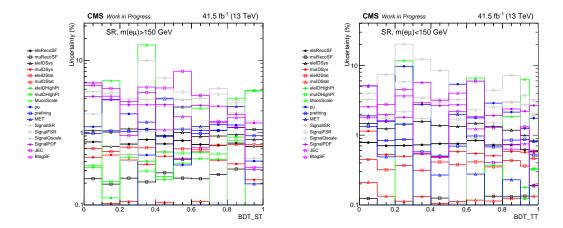
A comparison of different sources of systematic uncertainties of the background estimates in SR is shown in Figure 17.7.

A comparison of different sources of systematic uncertainties of the signal estimates in SR is shown in Figure 17.8.

Representative range of systematic uncertainties on background and signal MC samples are summarized in citeSysError. These uncertainties are extracted from the last bins of the BDT distribution.



**Figure 17.7:** Distributions of relative uncertainties on total expected backgrounds as a function of BDT output in ST enriched SR (left), TT enriched SR (right). Luminosity and normalization uncertainties are not included in these plots. JES, JER and HEM are combined into "JEC". Sources of b-tagging uncertainties listed in Table 17.1 are combined into "BtagSF".



**Figure 17.8:** Distributions of relative uncertainties on signal ( $C_{e\mu tu}^{vector}$  is used as an example) as a function of BDT output in ST enriched SR (left), TT enriched SR (right). Luminosity and normalization uncertainties are not included in these plots. JES, JER and HEM are combined into "JEC". Sources of b-tagging uncertainties listed in Table 17.1 are combined into "BtagSF".

## Chapter 18

#### **Statistical Analysis**

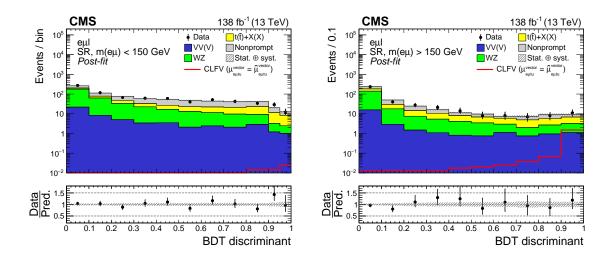
#### 18.1 Profile Likelihood Fit

A binned likelihood function  $\mathcal{L}(\mu,\theta)$  is constructed to perform the statistical analysis on the BDT discriminator distributions. The parameter of interest (POI), denoted by  $\mu$ , is the signal strength that governs the cross section of the ST and TT signals simultaneously. All the uncertainties are incorporated into the likelihood function as nuisance parameters, denoted by  $\theta$ . The uncertainties that affect the shape of the BDT discriminator distributions are considered with Gaussian distributions while other uncertainties that only affect the normalizations are considered with log-normal distributions.

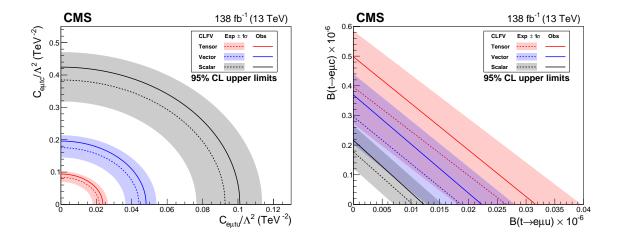
To control the systematic uncertainties, a profile likelihood fit is performed simultaneously in six regions (three data-taking years and two signal regions) by maximizing the likelihood function  $\mathcal{L}(\hat{\mu},\hat{\theta})$ . Both  $\hat{\mu}$  and  $\hat{\theta}$  are the maximum likelihood estimators for the signal strength and nuisance parameters, respectively. The scaling of the signal for the purpose of a better visualization is optimized based on "VecU" signal, and it is kept the same for the other signals to compare their cross sections relative to each other. The post-fit distributions of the BDT discriminator are shown in Fig. 18.1-??. The most prominent uncertainties affecting the likelihood fit are the statistical uncertainties on MC samples.

#### 18.2 Upper Limits

The results for the one-dimensional limits are summarized in Table 18.1. Assuming a linear relationship between  $\mathcal{B}(t\to e\mu c)$  and  $\mathcal{B}(t\to e\mu c)$  in the case of nonvanishing signals, the two-dimensional limits can also be obtained through interpolation (see Fig. 18.2). This analysis constitutes the most stringent limits on these processes to date.



**Figure 18.1:** Distributions of the posterior BDT discriminator distributions for the TT-enriched SR (left) and the ST-enriched SR (right). Signals are generated with vector-like operator involving an Up quark. The three data-taking years are aggregated for better visualization.



**Figure 18.2:** Two-dimensional upper limits on the Wilson coefficients (left) and the branching ratios (right).

CLFV	Lorentz	${\rm C_{e\mu tq}/\Lambda^2~(TeV^{-2})}$		$\mathcal{B}(t  o e\muq)  imes 10^{-6}$	
coupling	structure	exp (68% range)	obs	exp (68% range)	obs
eµtu	tensor	0.022 (0.018–0.026)	0.024	0.027 (0.018–0.040)	0.032
	vector	0.044 (0.036–0.054)	0.048	0.019 (0.013-0.028)	0.022
	scalar	0.093 (0.077–0.114)	0.101	0.010 (0.007–0.016)	0.012
eµtc	tensor	0.084 (0.069–0.102)	0.094	0.396 (0.272–0.585)	0.498
	vector	0.175 (0.145–0.214)	0.196	0.296 (0.203-0.440)	0.369
	scalar	0.385 (0.318-0.471)	0.424	0.178 (0.122–0.266)	0.216

**Table 18.1:** Upper limit on the LFV signal using the full Run 2 data set.

### Part IV

# Outlook for CLFV Searches Using Top Quarks



## **Inclusive Signal Generation**

- 19.1 UFO Model
- 19.2 EFT Reweighting

# 

### **Object and Event Selection**

- 20.1 Object Selection
- 20.2 Event Selection

# Chapter 21

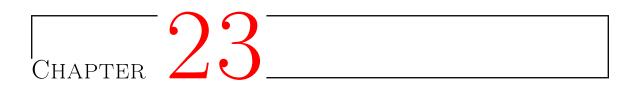
### **Expected Sensitivity**

- 21.1 Asimov Fit
- 21.2 Expected Upper Limits

# Chapter 22

#### **Run-2 Combination**

- 22.1 Correlation Scheme
- 22.2 Minimal Flavor Violation Interpretation



## **Summary and Conclusions**

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## List of Trigger Paths

**Table A.1:** Triggers used to record events during data taking in 2016.

Dataset	Trigger Path			
	HLT_lsoMu22_eta2p1, HLT_lsoTkMu22_eta2p1			
SingleMuon	HLT_lsoMu24, HLT_lsoTkMu24			
	HLT_Mu50, HLT_TkMu50, HLT_Mu45_eta2p1			
	HLT_Ele25_eta2p1_WPTight_Gsf			
	HLT_Ele27_WPTight_Gsf			
SingleElectron	HLT_Ele27_eta2p1_WPTight_Gsf			
SingleLlectron	HLT_Ele32_eta2p1_WPTight_Gsf			
	HLT_Ele105_CaloIdVT_GsfTrkIdT			
	HLT_Ele115_CaloldVT_GsfTrkIdT			
	HLT_Mu17_TrklsoVVL_Mu8_TrklsoVVL			
	HLT_Mu17_TrklsoVVL_TkMu8_TrklsoVVL			
	HLT_TkMu17_TrklsoVVL_TkMu8_TrklsoVVL			
DoubleMuon	HLT_Mu17_TrklsoVVL_Mu8_TrklsoVVL_DZ			
	HLT_Mu17_TrklsoVVL_TkMu8_TrklsoVVL_DZ			
	HLT_TkMu17_TrklsoVVL_TkMu8_TrklsoVVL_DZ			
	HLT_Mu30_TkMu11, HLT_TripleMu_12_10_5			
	HLT_Ele23_Ele12_CaloIdL_TrackIdL_IsoVL_DZ			
	HLT_Ele16_Ele12_Ele8_CaloIdL_TrackIdL			
DoubleEG	HLT_DoubleEle33_CaloIdL_MW			
	HLT_DoubleEle33_CaloIdL_GsfTrkIdVL			
	${\sf HLT\_DoubleEle33\_CaloldL\_GsfTrkldVL\_MW}$			
	HLT_Mu23_TrklsoVVL_Ele8_CaloIdL_TrackIdL_IsoVL			
	HLT_Mu23_TrkIsoVVL_Ele8_CaloIdL_TrackIdL_IsoVL_DZ			
	HLT _Mu8 _ TrklsoVVL _ Ele23 _ CaloIdL _ TrackIdL _ IsoVL			
MuonEG	HLT_Mu30_Ele30_CaloIdL_GsfTrkIdVL			
	HLT _Mu33 _Ele33 _CaloIdL _GsfTrkIdVL			
	HLT_DiMu9_Ele9_CaloIdL_TrackIdL			
	HLT _Mu8_ DiEle12 _ CaloIdL _ TrackIdL			

**Table A.2:** Triggers used to record events during data taking in 2017.

Dataset	Trigger Path		
SingleMuon	HLT_lsoMu24_eta2p1 HLT_lsoMu27 HLT_Mu50 HLT_OldMu100 HLT_TkMu100		
SingleElectron	HLT_Ele32_WPTight_Gsf_L1DoubleEG HLT_Ele35_WPTight_Gsf HLT_Ele115_CaloldVT_GsfTrkIdT		
DoubleMuon	HLT_Mu17_TrklsoVVL_Mu8_TrklsoVVL HLT_Mu17_TrklsoVVL_Mu8_TrklsoVVL_DZ HLT_Mu17_TrklsoVVL_Mu8_TrklsoVVL_DZ_Mass8 HLT_Mu17_TrklsoVVL_Mu8_TrklsoVVL_DZ_Mass3p8 HLT_Mu19_TrklsoVVL_Mu9_TrklsoVVL_DZ_Mass3p8 HLT_Mu37_TkMu27 HLT_TripleMu_12_10_5 HLT_TripleMu_10_5_5_DZ HLT_TripleMu_5_3_3_Mass3p8to60_DZ		
DoubleEG	HLT_Ele23_Ele12_CaloIdL_TrackIdL_IsoVL HLT_Ele16_Ele12_Ele8_CaloIdL_TrackIdL HLT_DoubleEle25_CaloIdL_MW HLT_DoubleEle33_CaloIdL_MW HLT_DiEle27_WPTightCaloOnly_L1DoubleEG		
MuonEG	HLT_Mu23_TrklsoVVL_Ele12_CaloIdL_TrackIdL_IsoVL HLT_Mu23_TrklsoVVL_Ele12_CaloIdL_TrackIdL_IsoVL_DZ HLT_Mu8_TrklsoVVL_Ele23_CaloIdL_TrackIdL_IsoVL_DZ HLT_Mu12_TrklsoVVL_Ele23_CaloIdL_TrackIdL_IsoVL_DZ HLT_Mu27_Ele37_CaloIdL_MV HLT_Mu37_Ele27_CaloIdL_MV HLT_DiMu9_Ele9_CaloIdL_TrackIdL HLT_DiMu9_Ele9_CaloIdL_TrackIdL HLT_DiMu8_DiEle12_CaloIdL_TrackIdL		

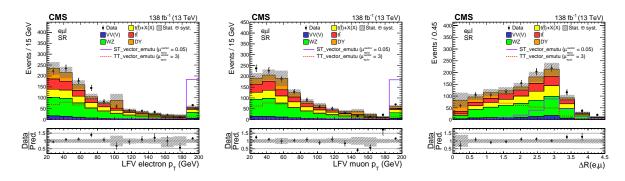
**Table A.3:** Triggers used to record events during data taking in 2018.

Dataset	Trigger Path
	HLT_IsoMu24
	HLT_IsoMu27
SingleMuon	HLT_Mu50
	HLT_OldMu100
	HLT_TkMu100
	HLT_Ele32_WPTight_Gsf
	HLT_Ele115_CaloldVT_GsfTrkIdT
EGamma	HLT_Ele23_Ele12_CaloIdL_TrackIdL_IsoVL
LGaiiiiia	HLT_Ele16_Ele12_Ele8_CaloIdL_TrackIdL
	HLT_DoubleEle25_CaloIdL_MW
	HLT_DiEle27_WPTightCaloOnly_L1DoubleEG
	HLT_Mu17_TrklsoVVL_Mu8_TrklsoVVL_DZ_Mass3p8
	HLT_Mu37_TkMu27
DoubleMuon	HLT_TripleMu_12_10_5
	HLT_TripleMu_10_5_5_DZ
	HLT_TripleMu_5_3_3_Mass3p8to60_DZ
	HLT_Mu23_TrklsoVVL_Ele12_CaloIdL_TrackIdL_IsoVL
	${\sf HLT\_Mu23\_TrklsoVVL\_Ele12\_CaloldL\_TrackldL\_lsoVL\_DZ}$
	HLT_Mu8_TrklsoVVL_Ele23_CaloIdL_TrackIdL_IsoVL_DZ
MuonEG	$HLT\_Mu12\_TrklsoVVL\_Ele23\_CaloldL\_TrackldL\_lsoVL\_DZ$
WidonEd	HLT_Mu27_Ele37_CaloIdL_MV
	HLT_Mu37_Ele27_CaloIdL_MV
	$HLT\_DiMu9\_Ele9\_CaloldL\_TrackIdL\_DZ$
	HLT_Mu8_DiEle12_CaloIdL_TrackIdL

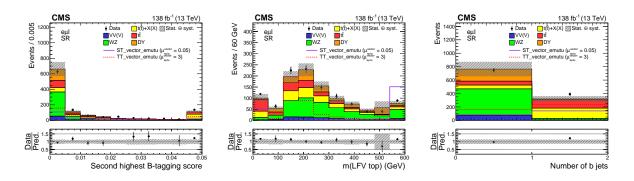
## Appendix B

#### Signal Region Distributions with MC simulation

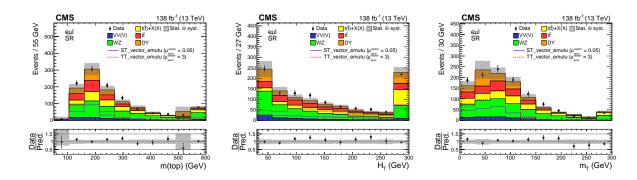
Distributions of various variables in SR, which are used in the BDT training. More details on these input features are described in section 16.2. The data are shown as filled points and the SM background predictions as histograms. The VV(V) background includes ZZ and triboson production, while the  $t\bar{t}+X(X)$  component includes  $t\bar{t}W$ ,  $t\bar{t}Z$ ,  $t\bar{t}H$ , tZq, and smaller backgrounds containing one or two top quarks plus a boson or quark. All backgrounds are estimated using MC simulation. The hatched bands indicate statistical and systematic uncertainties for the SM background predictions. The normalisation of the signal processes is chosen arbitrarily for improved visualisation.



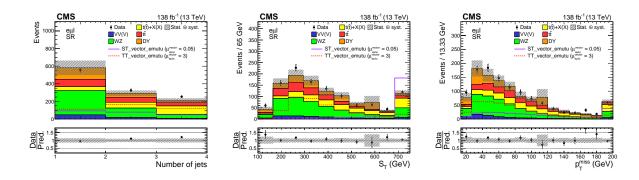
**Figure B.1:** Distributions of LFV electron  $p_T$  (left), LFV muon  $p_T$  (middle), and the opening angle between LFV electron and LFV muon (right).



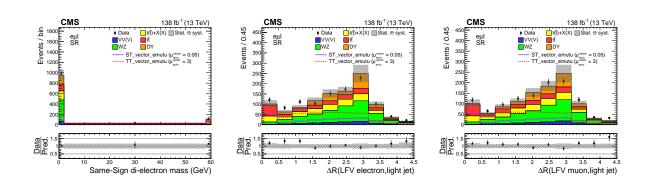
**Figure B.2:** Distributions of the second highest DEEPJET score (left), LFV top mass (middle), b jet multiplicity (right).



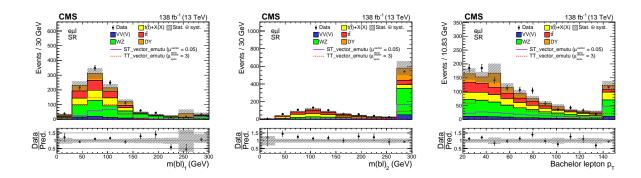
**Figure B.3:** Distributions of SM top quark mass (left), scalar sum of  $p_T$  of all jets (middle), and transverse mass of the W boson (right).



**Figure B.4:** Distributions of jet multiplicity (left), scalar sum of  $p_T$  of all jets and leptons (middle), and MET (right).



**Figure B.5:** Distributions of the same-sign di-electron mass (left), the opening angle between LFV electron and a light flavor jet (middle), and the opening angle between LFV muon and a light flavor jet (right).



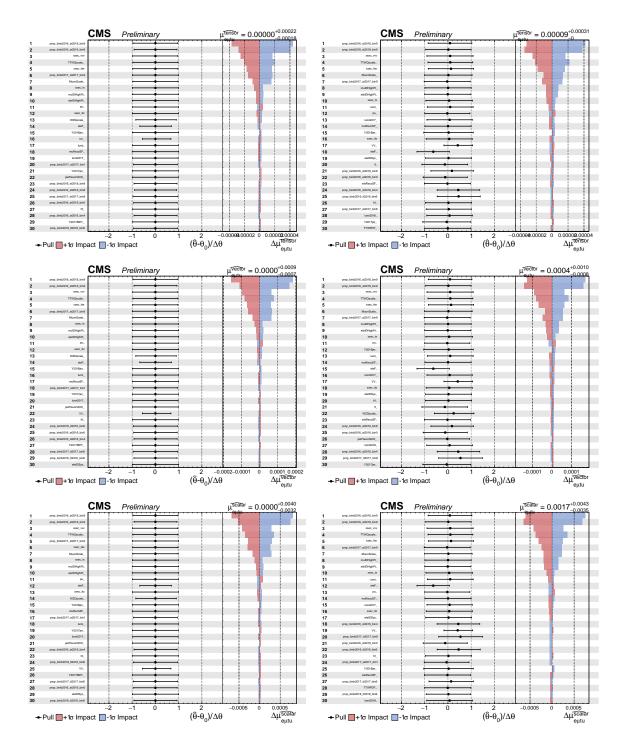
**Figure B.6:** Distributions of the mass of the first  $m_{b\ell}$  system (left), the mass of the second  $m_{b\ell}$  system (middle), and standalone lepton  $p_T$  (right).



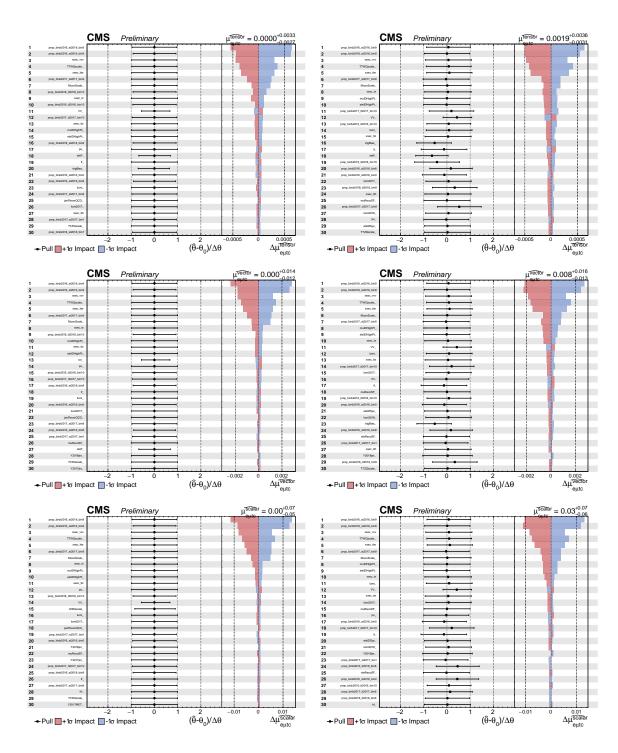
#### **Nuisance Parameter Impact**

The observed and expected ( $\mu_{exp}=0$ ) impacts of the nuisance parameters on the profile likelihood fit are shown in Figure C.1-C.2. They were computed using the following commands and plotted below for full run 2.

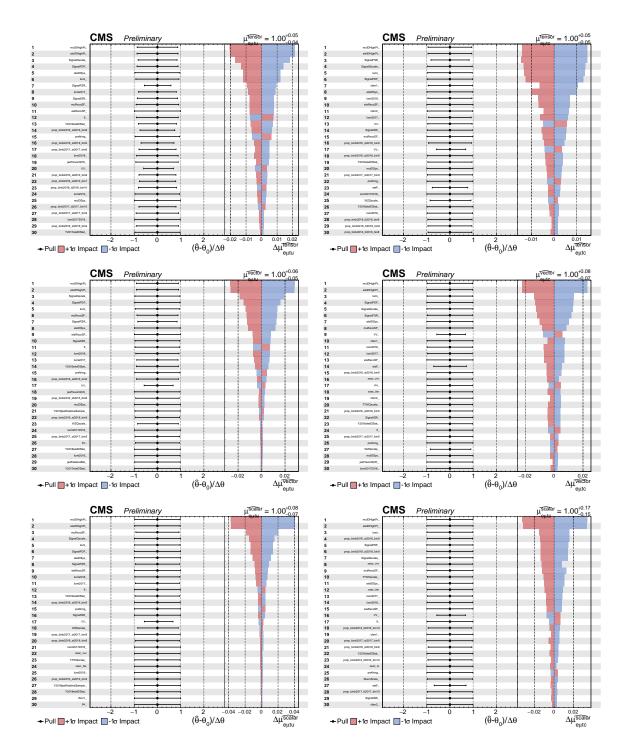
The expected  $(\mu_{exp} = 1)$  impacts of the nuisance parameters on the profile likelihood fit are shown in Figure C.3.



**Figure C.1:** Impacts of nuissance parameters for run II limit setting. From top to bottom:  $e\mu tu$ -tensor,  $e\mu tu$ -vector,  $e\mu tu$ -scalar. From left to right: expected impact (expected signal strength at 0), observed impact.



**Figure C.2:** Impacts of nuissance parameters for run II limit setting. From top to bottom:  $e\mu tc$ -tensor,  $e\mu tc$ -vector,  $e\mu tc$ -scalar. From left to right: expected impact (expected signal strength at 0), observed impact.



**Figure C.3:** Expected impact with an expected signal strength at 1. From top to bottom: tensor, vector, scalar. From left to right:  $e\mu tu$ ,  $e\mu tc$ .