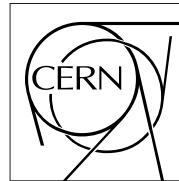


The Compact Muon Solenoid Experiment Analysis Note

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23 May 2017 (v9, 06 September 2019)

Measurement of the top-anti-top differential production cross section of high transverse momentum top quarks in the all-hadronic final state using the 2016 proton-proton collision data at $\sqrt{s} = 13$ TeV.

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Abstract

A measurement of the production cross section of high transverse momentum (p_T) top quark pairs is reported. The dataset was collected during 2016 with the CMS detector at the CERN LHC from proton-proton collisions at a center-of-mass energy of 13 TeV, and corresponds to an integrated luminosity of 35.9 fb^{-1} . The measurement uses events where either both top quark candidates decay hadronically and are reconstructed as large- R jets with $p_T > 400 \text{ GeV}$. The cross section is extracted differentially as a function of kinematic variables of the top quark or top quark pair system. The results are unfolded to the particle and parton levels, and are compared to various theoretical models. The measured cross section is significantly lower, by up to 40%, in the phase space of interest, compared

to the theory predictions, while the normalized differential cross sections are consistent between data and theory.

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1 Contents

2	1	Introduction	2
3	2	Samples	2
4	2.1	Data	2
5	2.2	Simulation	3
6	3	Trigger	5
7	4	Reconstruction and Selection	7
8	4.1	Object Reconstruction	7
9	4.2	Selection	7
10	4.3	Multivariate Discriminant	10
11	4.4	Parton level	13
12	4.5	Particle level	13
13	5	Signal Extraction	13
14	5.1	Inclusive cross section	14
15	5.2	Differential cross sections	15
16	6	Data vs Monte Carlo	21
17	7	Systematic Uncertainties	25
18	8	Fiducial Measurement	35
19	9	Unfolded Measurement	38
20	9.1	Parton Level	38
21	9.2	Particle Level	45
22	10	Summary	52
23	A	Data vs simulation with default MC normalization	57
24	B	NN Input Variables	60
25	C	Control Distributions	64
26	D	Background Sensitivity to Pileup	68
27	E	Unfolding Tests	69
28	F	Simulated b tagging efficiencies	75
29	G	Correlation Matrices	75

30 1 Introduction

31 The top quark completes the third generation of quarks in the standard model (SM), and the
 32 precise knowledge of its properties is critical for the overall understanding of the theory. Mea-
 33 surements of the top-anti-top quark pair ($t\bar{t}$) production cross section confront the predictions
 34 from quantum chromodynamics (QCD) and have the potential to constrain the QCD param-
 35 eters, while being sensitive to physics beyond the SM. Also, the $t\bar{t}$ production process is a
 36 dominant SM background to searches for new physics phenomena and therefore its precise
 37 knowledge is essential for new discoveries.

38 The large $t\bar{t}$ yield expected in proton-proton (pp) collisions at the CERN LHC allows to perform
 39 measurements of the $t\bar{t}$ production rate in a large phase space, and, more importantly, differ-
 40 entially, as a function of the $t\bar{t}$ kinematic properties. Such measurements have been performed
 41 by the ATLAS [1–6] and CMS [7–15] Collaborations at 7, 8, and 13 TeV center-of-mass energies,
 42 under the hypothesis of the resolved final state, where the decay products of the $t\bar{t}$ pair can
 43 be reconstructed individually. This hypothesis is valid for top quark transverse momenta, p_T ,
 44 up to approximately 500 GeV. However, at higher p_T ($p_T/m \approx 1$), the top quark decay prod-
 45 ucts are highly collimated (“boosted”) and they can no longer be reconstructed separately. In
 46 order to explore the highly boosted phase space, hadronic top quark decays are reconstructed
 47 as large-radius jets. Previous efforts in this domain by the ATLAS [16, 17] and CMS [18–20]
 48 Collaborations confirm that it is feasible to perform precise differential measurements of the $t\bar{t}$
 49 production and have also shown interesting deviations from the theory predictions.

50 In this note, a measurement of the differential boosted $t\bar{t}$ production cross section in the hadronic
 51 final state is presented, using pp collisions at $\sqrt{s} = 13$ TeV recorded with the CMS detector
 52 during the 2016 LHC run and amounting to a total integrated luminosity of 35.9 fb^{-1} . In the
 53 hadronic decay channel, each W boson arising from the top quark decays into a pair of light
 54 quarks. As a result, the final state consists of at least six partons (more are possible due to
 55 initial- and final-state radiation), two of which are b quarks. Due to the high boost consid-
 56 ered in this measurement ($p_T > 400$ GeV), the top quarks are reconstructed unambiguously as
 57 large-radius jets and the final state consists of at least two such jets.

58 This note is organized as follows: section 2 describes the data and Monte Carlo samples used
 59 in the analysis and section 3 discusses the triggers and the measurement of the corresponding
 60 efficiency. Then, section 4 presents the details of the jet reconstruction and the event selection.
 61 The signal extraction is discussed in section 5 and a comparison between data and simulation is
 62 reported in section 6. The systematic uncertainties are discussed in section 7, while the results
 63 are presented in sections 8 and 9. Finally, section 10 summarizes the results.

64 2 Samples

65 In this section we describe the data and Monte Carlo samples that are used in the analysis.

66 2.1 Data

67 The collision events used for the measurement of the $t\bar{t}$ cross section have been collected with
 68 the triggers described in Section 3 that are part of the JetHT primary dataset. Table 1 lists
 69 the samples that correspond to different data-taking eras and have been reconstructed in the
 70 03Feb2017 reprosessing. The good Run and luminosity section list used is contained in the
 71 certification file Cert_271036-284044_13TeV_23Sep2016ReReco_Collisions16_JSON.txt.
 72 The total integrated luminosity of the analyzed data is 35.9 fb^{-1} .

⁷³ In addition to the data from the JetHT dataset, we have used the SingleMuon dataset for the
⁷⁴ measurement of the trigger efficiency. The eras and run ranges are the same as the ones in
⁷⁵ Table 1.

Table 1: Data samples.

Sample	Run range	Luminosity (pb^{-1})
/JetHT/Run2016B-03Feb2017_ver2-v2/MINIAOD	273150-275376	5750
/JetHT/Run2016C-03Feb2017-v1/MINIAOD	275656-276283	2573
/JetHT/Run2016D-03Feb2017-v1/MINIAOD	276315-276811	4242
/JetHT/Run2016E-03Feb2017-v1/MINIAOD	276947-277420	4025
/JetHT/Run2016F-03Feb2017-v1/MINIAOD	277932-278808	3105
/JetHT/Run2016G-03Feb2017-v1/MINIAOD	278820-280385	7576
/JetHT/Run2016H-03Feb2017_ver2-v1/MINIAOD	281613-284035	8435
/JetHT/Run2016H-03Feb2017_ver3-v1/MINIAOD	284036-284044	216

⁷⁶ 2.2 Simulation

⁷⁷ Monte Carlo simulation is used to generate samples for the $t\bar{t}$ signal and to model the kine-
⁷⁸ matic distributions of some of the background processes. Samples of simulated $t\bar{t}$ events have
⁷⁹ been generated at next-to-leading order (NLO) in QCD using POWHEG v2 [21–25], assuming
⁸⁰ a top quark mass of $m_t = 172.5 \text{ GeV}$. Single top quark production in the t channel or in as-
⁸¹ sociation with a W boson are simulated at NLO with POWHEG [26]. The production of W or
⁸² Z bosons in association with jets (+jets), as well as QCD multijet events, are simulated with
⁸³ MG5_AMC@NLO [27] at leading order (LO), with the MLM matching algorithm [28].

⁸⁴ All simulated events are processed with PYTHIA 8.212 [29, 30] for modeling of the parton show-
⁸⁵ ering, hadronization, and underlying event (UE). The NNPDF 3.0 [31] Parton Distribution
⁸⁶ Functions (PDF) are used throughout, and the CUETP8M1 UE tune [32] is used for all processes
⁸⁷ except for the $t\bar{t}$, $t\bar{t}H$ and single top quark processes, for which the tune CUETP8M2T4 [33] is
⁸⁸ used. The Simulation of the CMS detector response is based on GEANT4 [34]. Additional pp
⁸⁹ interactions in the same or neighbouring bunch crossings (pileup) are simulated with PYTHIA
⁹⁰ and overlaid with generated events according to the pileup distribution measured in data.

⁹¹ The various simulated processes are normalized to the best known theoretical cross sections,
⁹² namely the $t\bar{t}$, +jets, and single top quark samples are normalized to NNLO precision in QCD [35–
⁹³ 37].

⁹⁴ The measured cross sections for the $t\bar{t}$ process are compared to theoretical predictions provided
⁹⁵ by the following Monte Carlo models: POWHEG combined with PYTHIA for the parton show-
⁹⁶ ering, as described above, or combined with HERWIG ++ [38] and the corresponding EE5C UE
⁹⁷ tune [39]. In addition, $t\bar{t}$ events were also generated with MC@NLO [27] combined with PYTHIA
⁹⁸ for the parton showering.

⁹⁹ In the first part of Table 2 we show the signal samples, while in the second part we show the
¹⁰⁰ background ones that include QCD multijet production, associated production of vector bosons
¹⁰¹ (W^\pm, Z) with jets, and single-top production. The list shows the total number of events ana-
¹⁰² lyzed, including all samples of the same kind (nominal, extensions, backup). The reconstruc-
¹⁰³ tion of the Monte Carlo samples belongs to the era RunIIISummer16MiniAODv2-PUMoriond17_80X_mcRun2_asy-
¹⁰⁴ and we have used the MINIAODSIM data tier. The reported cross sections have been used in
¹⁰⁵ the normalization of the various processes in the data vs MC comparison plots.

Table 2: Monte Carlo samples.

Sample	Events ($\times 10^6$)	σ (pb)
TT_TuneCUETP8M2T4_13TeV-powheg-pythia8, backup	153.4	832
TTJets_TuneCUETP8M2T4_13TeV-amcatnloFXFX-pythia8, backup	87.9	832
TT_TuneEE5C_13TeV-powheg-herwigpp, ext2, ext3	57.7	832
TT_hdampDOWN_TuneCUETP8M2T4_13TeV-powheg-pythia8, ext1	57.9	832
TT_hdampUP_TuneCUETP8M2T4_13TeV-powheg-pythia8, ext1	58.2	832
TT_TuneCUETP8M2T4down_13TeV-powheg-pythia8, ext1	58.3	832
TT_TuneCUETP8M2T4up_13TeV-powheg-pythia8, ext1	58.9	832
TT_TuneCUETP8M2T4_13TeV-powheg-fsrdown-pythia8, ext1, ext2	155.7	832
TT_TuneCUETP8M2T4_13TeV-powheg-fsrup-pythia8, ext1, ext2	152.6	832
TT_TuneCUETP8M2T4_13TeV-powheg-isrdown-pythia8, ext1, ext2	148.5	832
TT_TuneCUETP8M2T4_13TeV-powheg-isrup-pythia8_ext1, ext2	156.5	832
TT_TuneCUETP8M2T4_mtop1665_13TeV-powheg-pythia8, ext1, ext2, backup	19.4	832
TT_TuneCUETP8M2T4_mtop1715_13TeV-powheg-pythia8	19.6	832
TT_TuneCUETP8M2T4_mtop1735_13TeV-powheg-pythia8	19.4	832
TT_TuneCUETP8M2T4_mtop1755_13TeV-powheg-pythia8, ext1, ext2	59.4	832
TT_TuneCUETP8M2T4_mtop1785_13TeV-powheg-pythia8	16.4	832
QCD_HT200to300_TuneCUETP8M1_13TeV-madgraphMLM-pythia8, ext1	57.6	1.712e+6
QCD_HT300to500_TuneCUETP8M1_13TeV-madgraphMLM-pythia8, ext1	54.5	3.477e+5
QCD_HT500to700_TuneCUETP8M1_13TeV-madgraphMLM-pythia8, ext1	62.3	3.21e+4
QCD_HT700to1000_TuneCUETP8M1_13TeV-madgraphMLM-pythia8, ext1	45.4	6831
QCD_HT1000to1500_TuneCUETP8M1_13TeV-madgraphMLM-pythia8, ext1	15.1	1207
QCD_HT1500to2000_TuneCUETP8M1_13TeV-madgraphMLM-pythia8, ext1	11.8	119.9
QCD_HT2000toInf_TuneCUETP8M1_13TeV-madgraphMLM-pythia8, ext1	6.0	25.24
DYJetsToQQ_HT180_13TeV-madgraphMLM-pythia8	12.1	1187
WJetsToQQ_HT180_13TeV-madgraphMLM-pythia8	22.4	2788
ST_t-channel_top_4f_inclusiveDecays_13TeV-powhegV2-madspin-pythia8_TuneCUETP8M1	67.2	136.02
ST_t-channel_antitop_4f_inclusiveDecays_13TeV-powhegV2-madspin-pythia8_TuneCUETP8M1	38.8	80.95
ST_tW_top_5f_inclusiveDecays_13TeV-powheg-pythia8_TuneCUETP8M1_ext1	6.9	35.6
ST_tW_antitop_5f_inclusiveDecays_13TeV-powheg-pythia8_TuneCUETP8M1_ext1	6.9	35.6

106 3 Trigger

107 The trigger path employed for the collection of signal events uses single-jet L1 seeds that re-
 108 quire the presence of a jet with $p_T > 180 \text{ GeV}$. At HLT jets are reconstructed from (online)
 109 particle flow candidates using the anti-kt algorithm with distance parameter $R = 0.8$ and their
 110 mass, after trimming of soft particles, must be greater than 30 GeV . Interesting events are re-
 111 quired to have at least two such jets with $p_T > 280(200) \text{ GeV}$ for the leading (trailing) one.
 112 Finally, at least one of the two jets should be tagged as a b-jet, using the online CSV algorithm.
 113 The aforementioned trigger path ran unprescaled for the duration of the 2016 run, collecting an
 114 integrated luminosity of 35.9 fb^{-1} . A second, prescaled, path, using the same L1 seed, was also
 115 employed, with identical kinematic requirements but no b-tagging cut, which ran in parallel
 116 and collected an integrated luminosity of 1.67 fb^{-1} . This path is used for the selection of a
 117 control QCD sample, as described later. All the triggers described above are summarized in
 118 Table 3. Finally, it should be noted that the pileup profile of the prescaled control trigger is
 119 shifted to lower number of interactions (Fig. 1), because the path tended to collect more data
 120 towards the end of the fills when the instantaneous luminosity was lower.

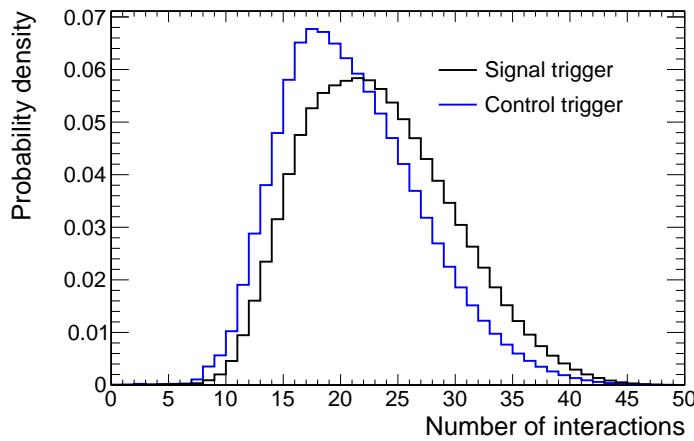


Figure 1: Pileup profile for the signal and control trigger paths.

Table 3: Summary of triggers used in the analysis.

Trigger	Purpose
L1_SingleJet180 OR L1_SingleJet200	L1 seed
HLT_AK8DiPFJet280_200_TrimMass30_BTagCSV_p20	signal HLT path
HLT_AK8DiPFJet280_200_TrimMass30	control HLT path

121 The efficiency of the signal trigger path is measured with respect to an orthogonal path that
 122 requires the presence of an isolated muon with $p_T > 27 \text{ GeV}$ (HLT_IsoMu27). Figure 2 shows
 123 the trigger efficiency as a function of the second jet p_T in events with at least two reconstructed
 124 jets, with at least one of them containing a b-tagged subjet. For details about the offline recon-
 125 struction see Section 4. The efficiency measured in data is compared to the simulated efficiency,
 126 showing an excellent agreement. The offline selection requires that the second jet p_T is greater
 127 than 400 GeV , which is at the beginning of the efficiency plateau.

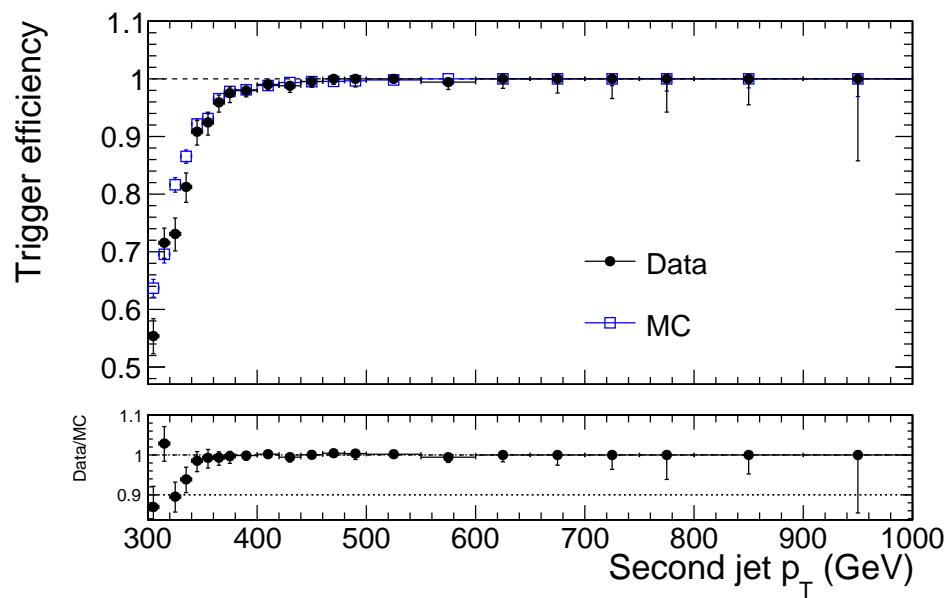


Figure 2: Trigger efficiency for the signal path of the analysis.

128 4 Reconstruction and Selection

129 In this section we present the objects used in the analysis, the multivariate method that dis-
 130 criminated $t\bar{t}$ events from the QCD multijet background, and we describe the event selection.

131 4.1 Object Reconstruction

132 The leptons (muons, electrons) used in the analysis come from the default reconstructed col-
 133 lections in CMS samples ('slimmedMuons' and 'slimmedElectrons') and must have
 134 $p_T > 20 \text{ GeV}$. Muons are required to pass the medium ID working point and electrons should
 135 pass the tight working point, while both lepton types should have a relative mini-isolation less
 136 than 0.1.

137 Jets are reconstructed from particle-flow (PF) candidates that have undergone charged-hadron
 138 subtraction (CHS) in order to suppress the contribution from multiple soft interactions in the
 139 same bunch crossing (pileup). The momentum 4-vectors of the PF candidates are clustered
 140 with the anti-kt algorithm with distance parameter $R = 0.8$, hence we refer to AK8 PFCHS
 141 jets. These jets are required to pass the tight jet ID. Furthermore, an algorithm is run to identify
 142 subjets with distance parameter $R = 0.4$ within the AK8 jets. Finally, the soft-drop technique
 143 is used in order to evaluate the mass of the AK8 jet with suppressed pileup contribution. For
 144 all the aforementioned algorithms we have used the default definitions in the CMS software
 145 and the default collections in the MINIAOD data and Monte Carlo samples. For the energy
 146 calibration of the AK8 jets we have used the recommended corrections by the JME POG in the
 147 80X_dataRun2_2016SeptRepro_v7 and 80X_mcRun2_asymptotic_2016_TrancheIV_v8 global
 148 tags.

149 The selection of AK8 jets that originate from the top decay relies on the identification of a b-jet
 150 within them. For this purpose, we use the CSVv2 b-tagging algorithm applied on the AK4
 151 subjets of each AK8 jet. In particular, we use the medium working point, which requires the
 152 value of the tagger to be greater than 0.8484.

153 Since leptons are also reconstructed as jets, we perform cross cleaning by removing each iden-
 154 tified lepton from the jet collection with geometrical matching in the $\eta - \phi$ space: if a jet has
 155 $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2} < 0.4$ from any accepted lepton candidate it is removed from the jet
 156 collection.

157 4.2 Selection

158 The baseline selection, summarized in Table 4 is common for all regions used in the analysis
 159 and it requires at least two jets in the event with $p_T > 400 \text{ GeV}$ and softDrop masses in the
 160 range $(50, 300) \text{ GeV}$. Also, a lepton veto is applied in order to minimize the probability to select
 161 leptonic top decays. Then, on top of the baseline selection, we define four specific regions
 162 (Table 4) based on the NN output (Section 4.3), the jets' softDrop masses, and the number of
 163 b-tagged subjets in each jet, that serve different analysis purposes. The signal region (SR) is
 164 where we perform the differential measurements and it requires both jets to have a b-tagged
 165 subjet, a tighter selection on the jets' masses, and a high mva value. Figure 3 shows the top
 166 decay mode of the selected $t\bar{t}$ events, where more than 95% come from the hadronic channel.
 167 The QCD control region (CR) is the same as the SR but with the b-tagging requirement reverted
 168 (the jets should not contain a b-tagged subjet) and it is used to get from data the shape of the
 169 QCD background for each variable of interest. Then, we employ the signal region A (SR_A),
 170 which is used to determine the normalization of the QCD background, and finally the signal
 171 region B (SR_B), which is used to constrain some of the signal modelling uncertainties. Figure 4

¹⁷² shows a cartoon of the signal regions on the plane defined by the NN output and the jet masses.

Table 4: Baseline selection requirements.

Observable	Requirement
N_{jets}	> 1
N_{leptons}	$= 0$
$p_{\text{T}}^{\text{jet}1,2}$	$> 400 \text{ GeV}$
$m_{SD}^{\text{jet}1,2}$	$(50, 300) \text{ GeV}$

Table 5: Selection requirements per analysis region.

Region	Trigger	Offline Requirements	Purpose
SR	signal	$\text{Base+NN} > 0.8 + 2\text{btags} + m_{SD}^{\text{jet}1,2} \in (120, 220) \text{ GeV}$	signal region
SR_A	signal	$\text{Base+NN} > 0.8 + 2\text{btags}$	QCD fit region
SR_B	signal	$\text{Base} + 2\text{btags} + m_{SD}^{\text{jet}1,2} \in (120, 220) \text{ GeV}$	signal systematics region
CR	control	$\text{Base+NN} > 0.8 + 0\text{btags} + m_{SD}^{\text{jet}1,2} \in (120, 220) \text{ GeV}$	QCD control region

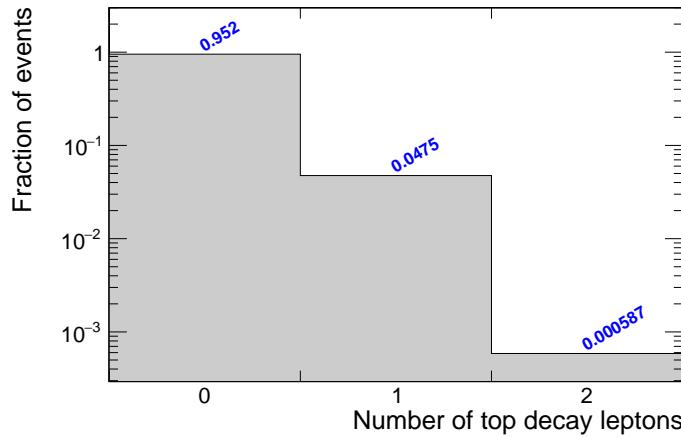


Figure 3: Distribution of $t\bar{t}$ decay modes after the signal selection of the analysis.

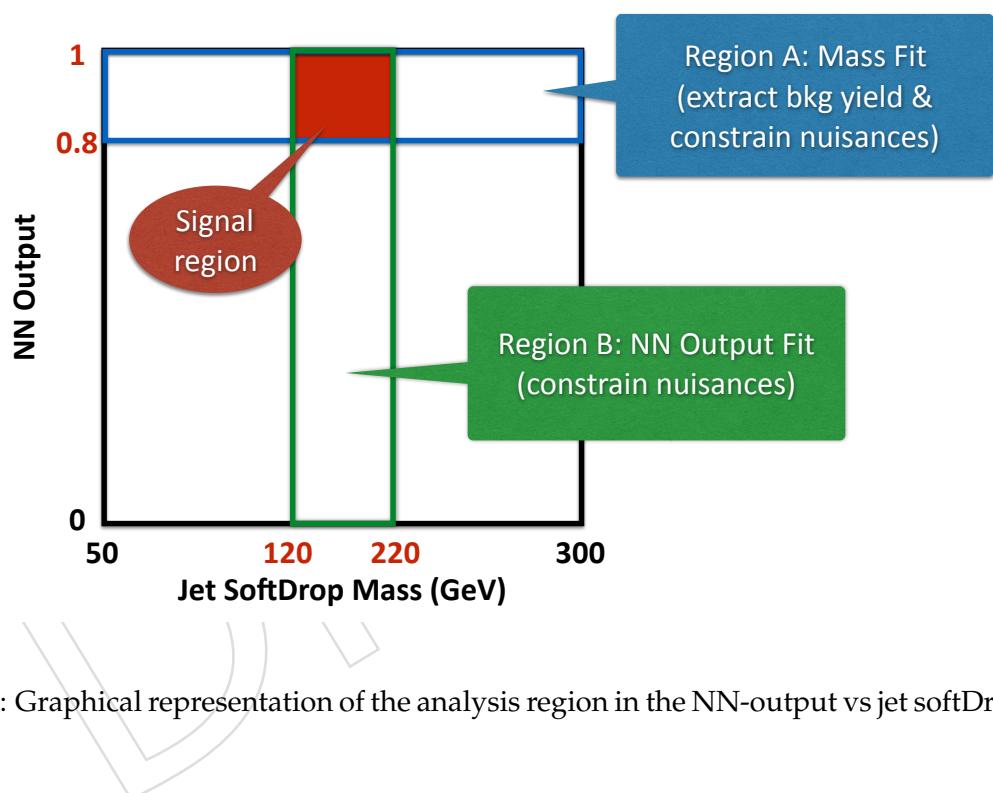


Figure 4: Graphical representation of the analysis region in the NN-output vs jet softDrop mass.

¹⁷³ **4.3 Multivariate Discriminant**

¹⁷⁴ In order to discriminate between events that come from $t\bar{t}$ decays and QCD multijet production
¹⁷⁵ we rely on variables that reveal the jet substructure. In particular, we use the "N-subjettiness"
¹⁷⁶ τ_N , defined as:

$$\tau_N = \frac{1}{\sum_k p_{T,k} R} \sum_k p_{T,k} \min\{\Delta R_{1,k}, \Delta R_{2,k}, \dots, \Delta R_{N,k}\}, \quad (1)$$

¹⁷⁷ where N denotes the reconstructed candidate subjets and k runs over the constituent particles
¹⁷⁸ in the jet. The variable $\Delta R_{i,k} = \sqrt{(\Delta y_{i,k})^2 + (\Delta \phi_{i,k})^2}$ is the angular distance between the can-
¹⁷⁹ didate subjet i and the particle k . The variable R is the characteristic jet radius ($R = 0.8$ in our
¹⁸⁰ case).

¹⁸¹ Since the signal final state ($t\bar{t}$ hypothesis) involves two jets with a top-quark decay signature,
¹⁸² we consider the N-subjettiness variables $\tau_{1,2,3}$ for both leading jets in the event, resulting in
¹⁸³ six discriminating variables per event. The distributions of these variables in $t\bar{t}$ and QCD
¹⁸⁴ simulated events are shown in Fig. 5, indicating that there is significant separating power in
¹⁸⁵ them. The linear correlation between the variables is shown in Fig. 6. In order to exploit fully
¹⁸⁶ the differences of the N-subjettiness variables we turn to multivariate discriminants, imple-
¹⁸⁷ mented in the TMVA package [40]. As a baseline we consider a simple Fisher discriminant,
¹⁸⁸ which is a linear combination of the variables. Then, a feed-forward neural network (NN)
¹⁸⁹ is constructed to enhance the discriminating power quantified by the integral of the receiver-
¹⁹⁰ operator-characteristic (ROC) curve. The network (Fig. 7) is composed of two hidden layers
¹⁹¹ with 16 and 4 nodes, respectively, each of one using a sigmoid activation function. The dis-
¹⁹² tribution of the NN output and the convergence of its training are shown in Fig. 8. As shown
¹⁹³ in Fig. 9, the NN is clearly better than the simple Fisher discriminant and it also outperforms
¹⁹⁴ slightly a Boosted Decision Tree composed of 500 trees and trained with the Gradient Boost
¹⁹⁵ method with shrinkage parameter equal to 0.1. More complicated NN architectures have not
¹⁹⁶ been found to improve the performance. The training is performed with events that pass the
¹⁹⁷ baseline selection and the MC samples are divided in two halves, one used for the training and
¹⁹⁸ one for the testing.

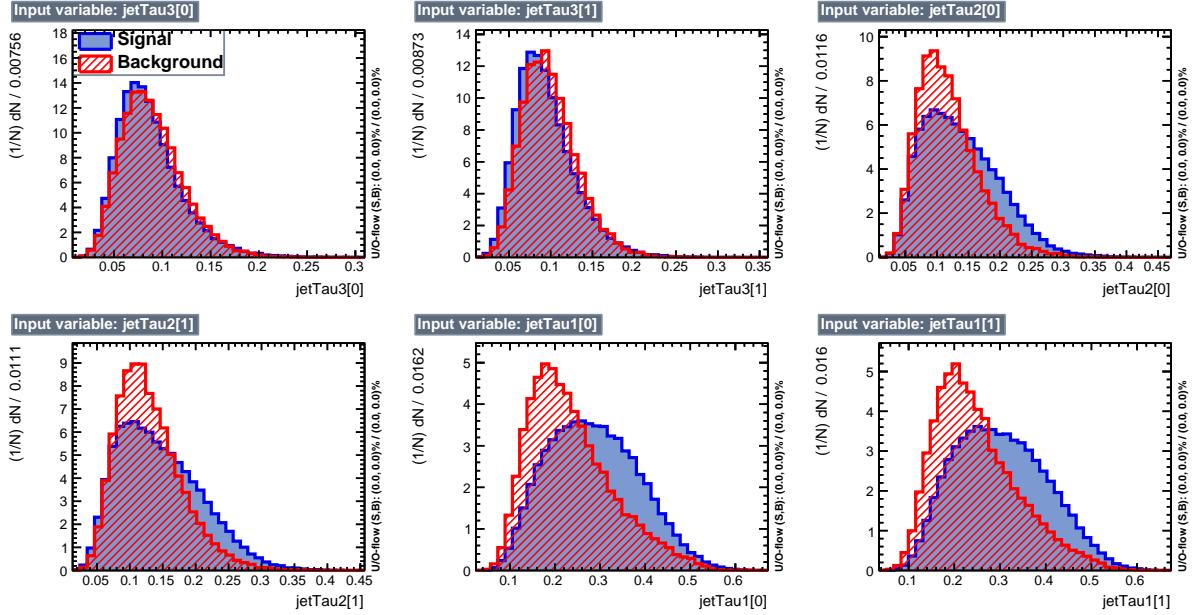


Figure 5: Discriminating variables used for the separation of $t\bar{t}$ from QCD events.

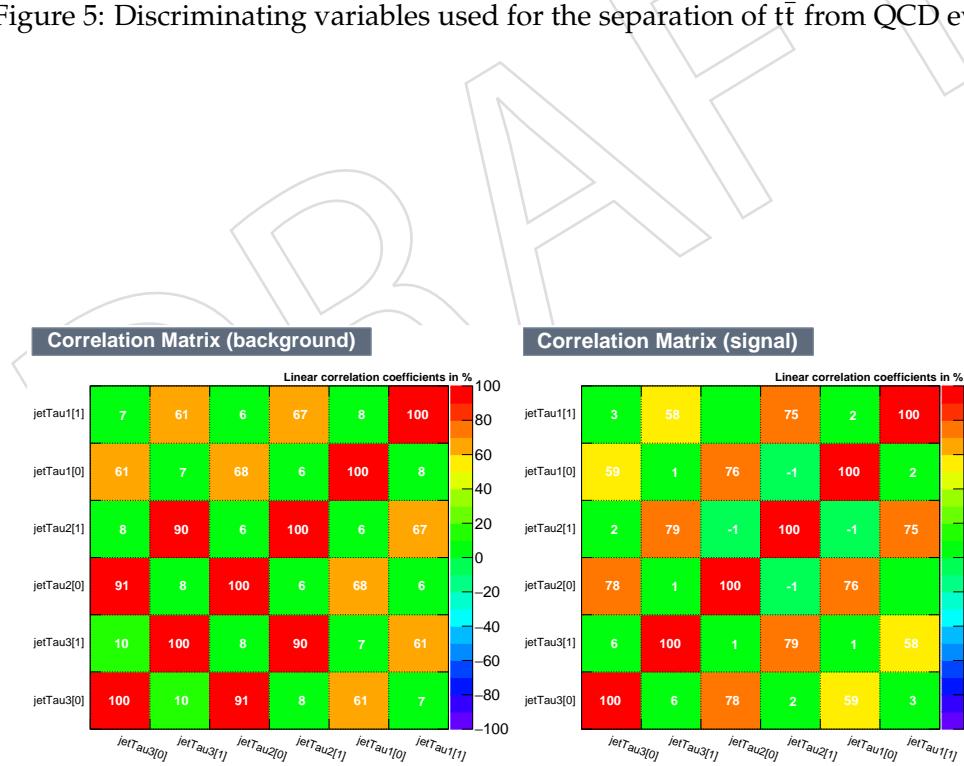


Figure 6: Linear correlation between the discriminating variables in background (left) and signal (right) events.

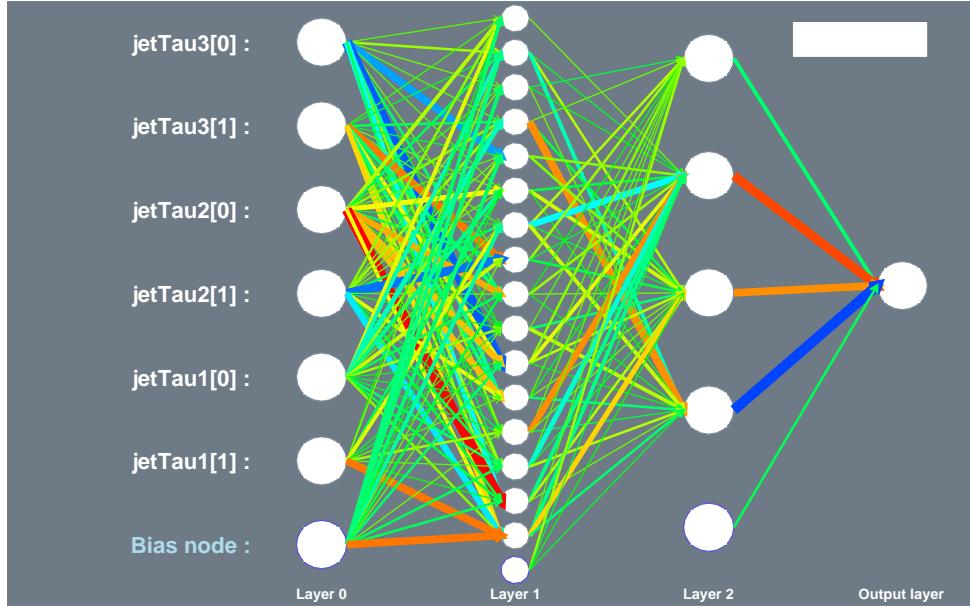


Figure 7: Neural network architecture.

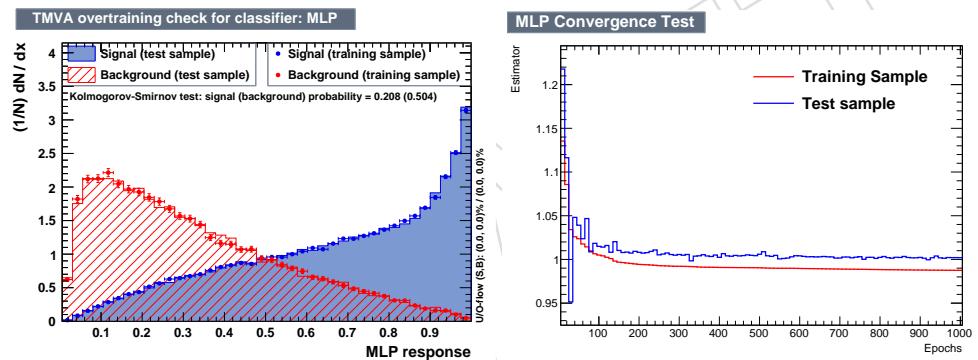


Figure 8: Output of the NN (left). Convergence of the NN training (right).

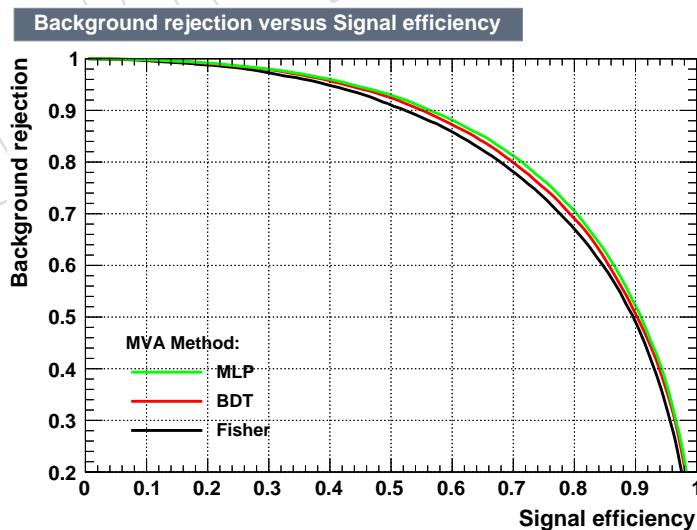


Figure 9: Performance of the multivariate discriminants in the form of a receiver-operator-characteristic curve.

199 **4.4 Parton level**

200 The partonic phase space to which we unfold the measurement is constrained by the kinematic
 201 requirements of the detector-level fiducial region. Namely, the top and anti-top partons must
 202 have $p_T > 400 \text{ GeV}$ and $|\eta| < 2.4$, while the invariant mass of the $t\bar{t}$ system must be greater
 203 than 800 GeV in order to avoid extreme events with high top p_T and very low $m_{t\bar{t}}$. These cuts
 204 are summarized in Table 6.

Table 6: Definition of parton-level phase space.

Observable	Requirement
$p_T^{t,\bar{t}}$	$> 400 \text{ GeV}$
$ \eta^{t,\bar{t}} $	< 2.4
$m_{t\bar{t}}$	$> 800 \text{ GeV}$

205 **4.5 Particle level**

206 The so-called "particle level" represents the state that consists of stable particles originating
 207 from the proton-proton collision, after the hadronization process, and before the interaction of
 208 these particles with the detector. The observables computed from the particles' momenta are
 209 thought to be better defined compared to the ones computed from parton information and ac-
 210 companied by smaller theoretical uncertainties. Also, the associated phase space is closer to the
 211 fiducial phase space of the measurement at detector level. In the context of this analysis, parti-
 212 cle jets are reconstructed from stable particles, excluding neutrinos, with the anti-kt algorithm
 213 of distance parameter $R = 0.8$, identical to the detector-level reconstruction. It should be noted
 214 that only particles originating from the primary interaction are considered. Subsequently, jets
 215 that are geometrically matched, within $\Delta R < 0.4$ in $\eta - \phi$ from generated leptons (i.e. from the
 216 leptonic decays of the W boson) are removed from the particle-jet collection. Finally, the two
 217 particle jets with the highest p_T are considered the particle-level top-quark candidates. In order
 218 to match as closely as possible the fiducial phase space, the same kinematic cuts are applied as
 219 for detector-level events. These requirements are summarized in Table 7.

Table 7: Definition of particle-level phase space.

Observable	Requirement
N_{jets}	> 1
$p_T^{\text{jet}1,2}$	$> 400 \text{ GeV}$
$ \eta^{\text{jet}1,2} $	< 2.4
$m_{SD}^{\text{jet}1,2}$	(120, 220) GeV
m_{jj}	$> 800 \text{ GeV}$

220 In order to verify the sanity of the adopted particle-level definition, in each event that passes
 221 the requirements above, the top candidates are matched within $\Delta R < 0.4$ in $\eta - \phi$ to the original
 222 top quarks at parton level. Figure 56 shows this efficiency, which varies between 96% and 98%,
 223 as a function of particle-level top p_T and η .

224 **5 Signal Extraction**

225 The, by far, dominant background in this analysis is the QCD multijet production, as there is
 226 a finite probability that ordinary jets, from single parton radiation, will mimic the topological
 227 substructure of a top-decay jet. With a combination of b-tagging requirements on the subjets

and n-subjettiness variables, we are able to suppress significantly the QCD background. In order to estimate the remaining contribution we employ a data-driven technique based on the assumptions that if the b-tagging requirement is reverted we a) get a pure QCD sample, and b) the jet kinematic properties are not affected.

5.1 Inclusive cross section

Before we attempt to extract differential cross sections, we first measure the inclusive, fiducial cross section. This is done in region SR_A that contains a QCD dominated sideband in the top candidate mass (softDrop mass of the leading jet) and allows a simultaneous fit for the $t\bar{t}$ signal and the QCD background yields. The fit is described by the equation below:

$$D_{SR_A}(m^t) = N_{t\bar{t}} T(m^t; k_{\text{scale}}, k_{\text{res}}) + N_{\text{qcd}}(1 + k_{\text{slope}} m^t) Q_{CR_A}(m^t) + N_{\text{bkg}} B(m^t), \quad (2)$$

which contains the shapes (templates) $T(m^t)$, $B(m^t)$ of the signal and the subdominant backgrounds, respectively, taken from the simulation, and the shape $Q(m^t)$ of QCD taken from the control sample in data (CR_A). The templates of the various components are shown in Figs. 10,11. To account for the difference observed in the closure test of QCD for the m^t variable (Fig. 12) we introduce the linear modification factor $(1 + k_{\text{slope}} m^t)$, inspired by the simulation, but with the slope parameter k_{slope} left free in the fit. Also free in the fit are the normalization factors $N_{t\bar{t}}$, N_{qcd} , and N_{bkg} . Finally, we introduce two more nuisance parameters in the $t\bar{t}$ simulation, k_{scale} and k_{res} that account for possible differences between data and simulation in the scale and resolution of the m^t parameter. The fit model is imported to the RooFit package and the fit result is shown in Fig. 13 while the fitted parameters are summarized in Table 8. We observe that the fitted $t\bar{t}$ yield (6238) is significantly lower than the expectation (9604), which implies that the fiducial cross section is $\approx 35\%$ lower compared to the Powheg+Pythia8 prediction. The nuisance parameters related to the m^t scale and resolution are consistent with one and the slope of the QCD modification factor $(5.7 \pm 1.4) \times 10^{-3}$ is very close to the value from the QCD simulation $((5.4 \pm 1.2) \times 10^{-3})$. Finally, despite the large uncertainty, the yield of the subdominant backgrounds (400 ± 247) is very close to the Monte Carlo prediction (380) in Table 9.

The fitted $t\bar{t}$ yield can be converted to a fiducial cross section $\sigma_{\text{fid}} = \frac{N_{t\bar{t}}}{\mathcal{L}}$. For an estimate of the systematic uncertainties, we repeat the measurement, independently, for each of the sources of uncertainty described in section 7. For each variation, a new $t\bar{t}$ template is introduced and the fit is repeated. The independent results are shown in Fig. 14 and the resulting cross section is $\sigma = 174.7 \pm 5.1(\text{fit})^{+3.3}_{-5.1}(\text{syst.}) \pm 4.2(\text{lumi.})$. The measured cross section is found to be a factor $r = 0.635$ lower than the theoretical prediction (Powheg+Pythia8). This factor is used to scale down the $t\bar{t}$ contribution in the data vs simulation comparisons.

Table 8: Results of the fit in SR_A .

Parameter	Value	Error
k_{res}	0.960	0.026
k_{scale}	1.002	0.002
k_{slope}	5.7e-03	1.4e-03
N_{bkg}	400	255
N_{qcd}	4539	247
$N_{t\bar{t}}$	6238	181

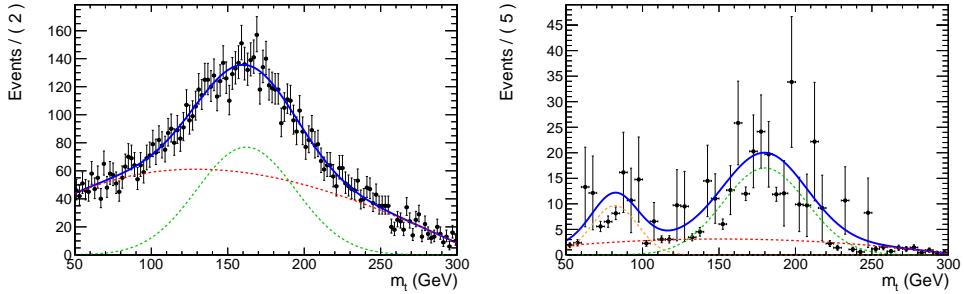


Figure 10: Templates of QCD (left), taken from data, and of the subdominant backgrounds (right), taken from the simulation. The different lines show the individual components (frozen in the fit) used to describe the shapes. The QCD shape is composed of a smooth polynomial and a Gaussian, while the shape of the subdominant backgrounds contains a smooth polynomial and two Gaussians (one describes the W resonance from the single top and WJets processes and the other describes the broader peak from the kinematic selections).

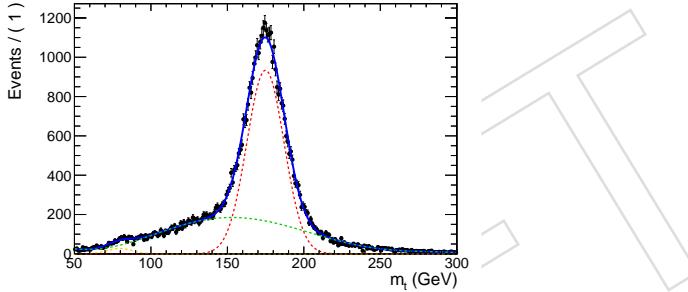


Figure 11: Template of the $t\bar{t}$ signal taken from the simulation. The different lines show the individual components (frozen in the fit) used to describe the shape. The shape consists of a smooth polynomial and two Gaussians (one describes the W resonance from unmerged top decays and the other describes the fully merged top resonance).

261 5.2 Differential cross sections

262 The $t\bar{t}$ cross section is also reported differentially, in the signal region SR as a function of several
 263 variables: the leading and second top p_T and $|y|$, and the $t\bar{t}$ mass, p_T , and rapidity. For the
 264 derivation of the differential cross sections, the background contributions are subtracted from
 265 the data:

$$S(x) = D(x) - R_{yield} N_{qcd} Q(x) - B(x), \quad (3)$$

266 where $x = p_T^{t1,2}, |y^{t1,2}|, m^{t\bar{t}}, p_T^{t\bar{t}}, y^{t\bar{t}}$, $S(x)$ is the signal, $D(x)$ is the measured distribution in
 267 data, $Q(x)$ is the QCD shape, $B(x)$ is the subdominant backgrounds' contribution (both the
 268 shape and the normalization are taken from the simulation), R_{yield} is the yield ratio between
 269 the signal region (SR) and the fit region (SR_A), and N_{qcd} is the fitted number of QCD events in
 270 SR_A .

271 The two elements that need to be determined from data are the shape $Q(x)$ of the QCD back-
 272 ground as a function of an observable of interest x , and the absolute normalization N_Q . The
 273 QCD template $Q(x)$ is taken from the QCD control sample by applying the signal region selec-
 274 tion with reverted b-tagging requirement (none of the leading AK8 jets is allowed to contain
 275 a b-tagged subjet). Figures 15, 16, 17 show the closure test in MC as a function of jet and di-

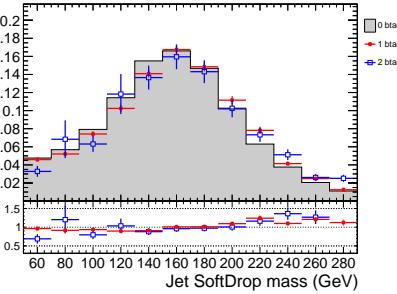


Figure 12: Closure test in the QCD simulation for the shape of the m^t variable in the three possible b-tagging requirements (none, exactly one, or both jets contain a b-tagged subjet).

276 jet kinematic variables. We observe that, within the statistical precision of the simulation, the
 277 shapes are compatible, regardless of the b-tagging requirement. Moreover, Figs. 19,20 show
 278 that indeed the 0-btag sample has negligible $t\bar{t}$ contamination.

279 The normalization of the QCD background is determined from the fit to the data in SR_A . How-
 280 ever, since this is an extended signal region, a transfer factor $R_{\text{yield}} = N^{\text{SR}} / N^{SR_A}$ is needed in
 281 order to get the QCD normalization in the signal region. Figure 18 shows a closure test per-
 282 formed in **QCD Monte Carlo events**, where the value of R_{yield} is independent of the b-tagging
 283 requirement (within the statistical precision of the simulation), and therefore can be taken from
 284 the QCD control sample ($R_{\text{yield}} = N^{\text{CR}} / N^{CR_A}$).

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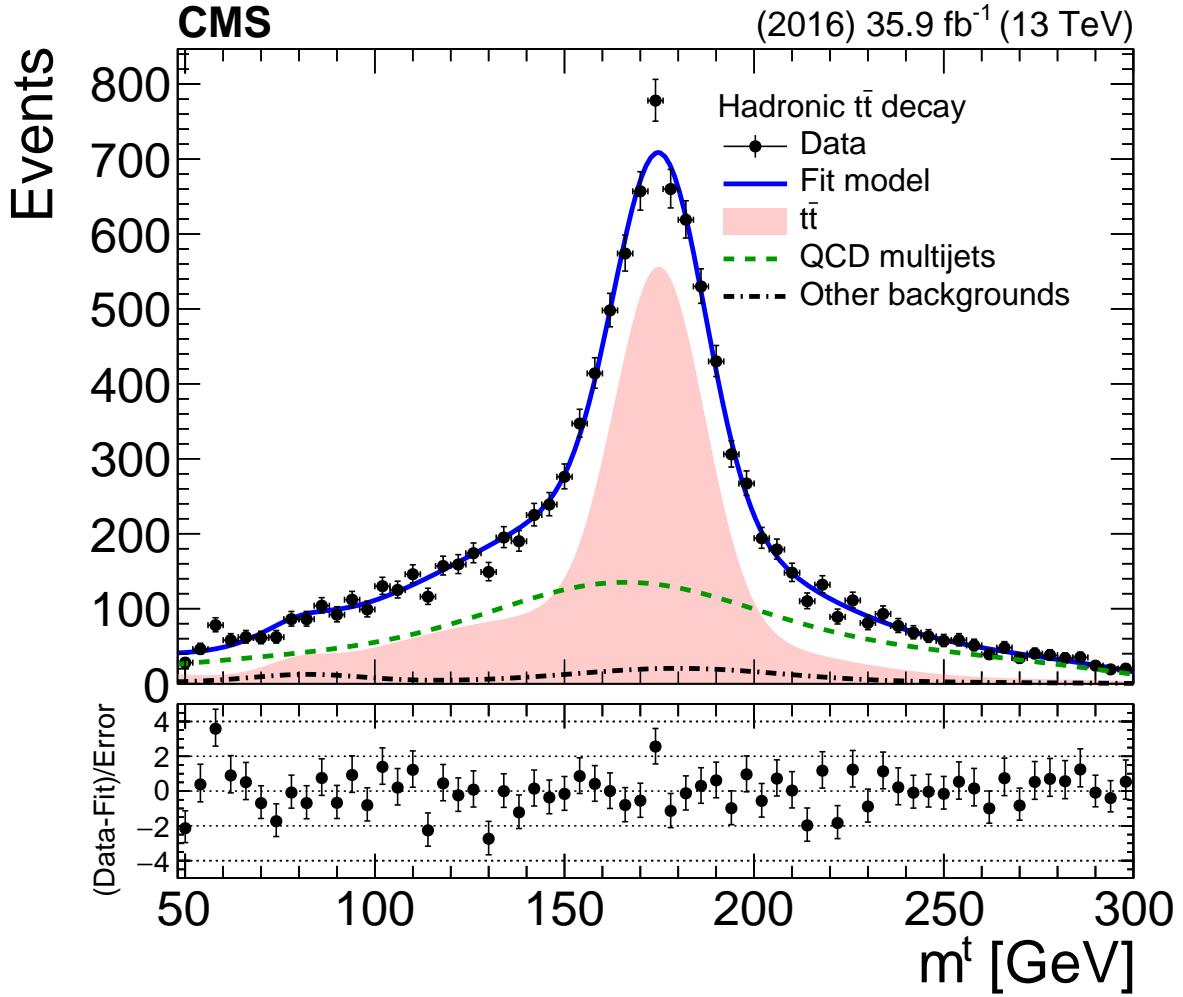


Figure 13: Result of the template fit on data. The red line shows the $t\bar{t}$ contribution, the green line shows the QCD, and the brown line shows the subdominant backgrounds.

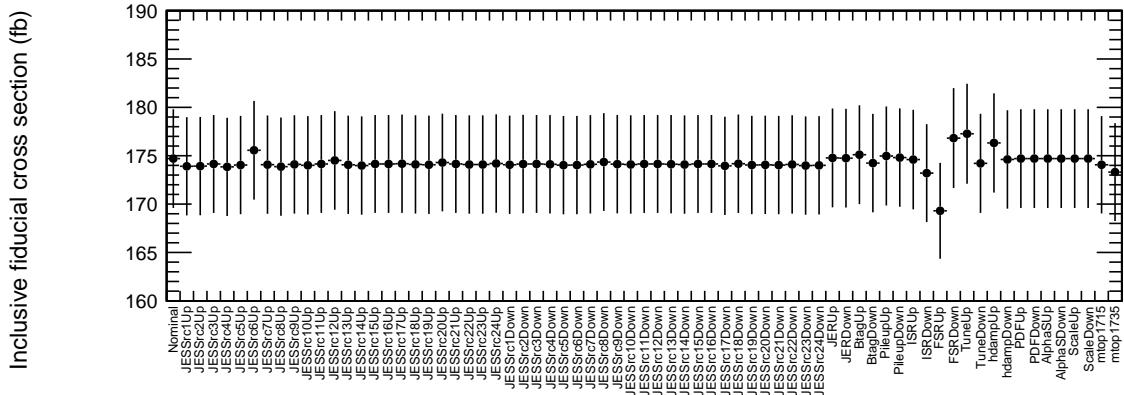


Figure 14: Measurements of the inclusive, fiducial $t\bar{t}$ cross section for the nominal signal simulation and all the systematic variations.

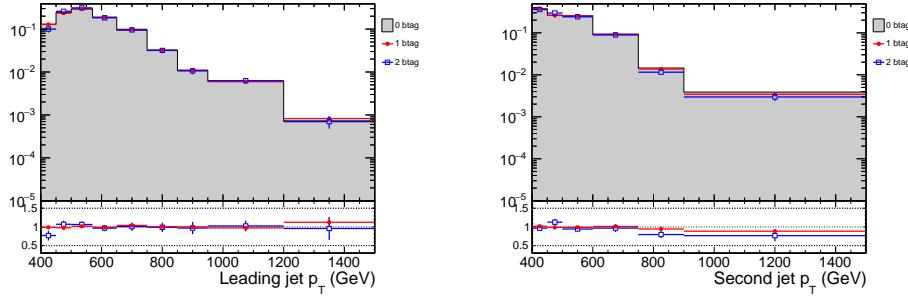


Figure 15: Closure test for the data-driven QCD prediction method for the shape of the top p_T variables.

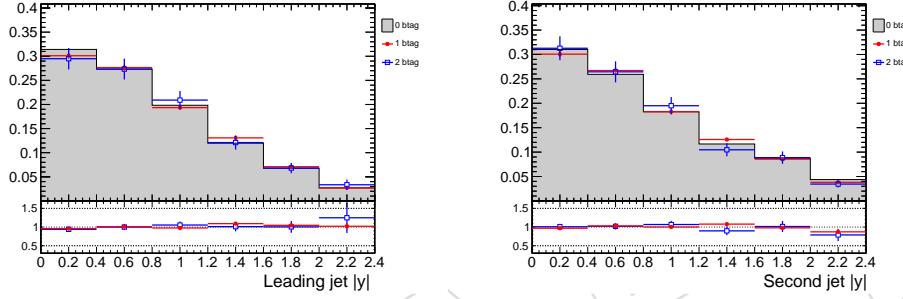


Figure 16: Closure test for the data-driven QCD prediction method for the shape of the top $|y|$ variables.

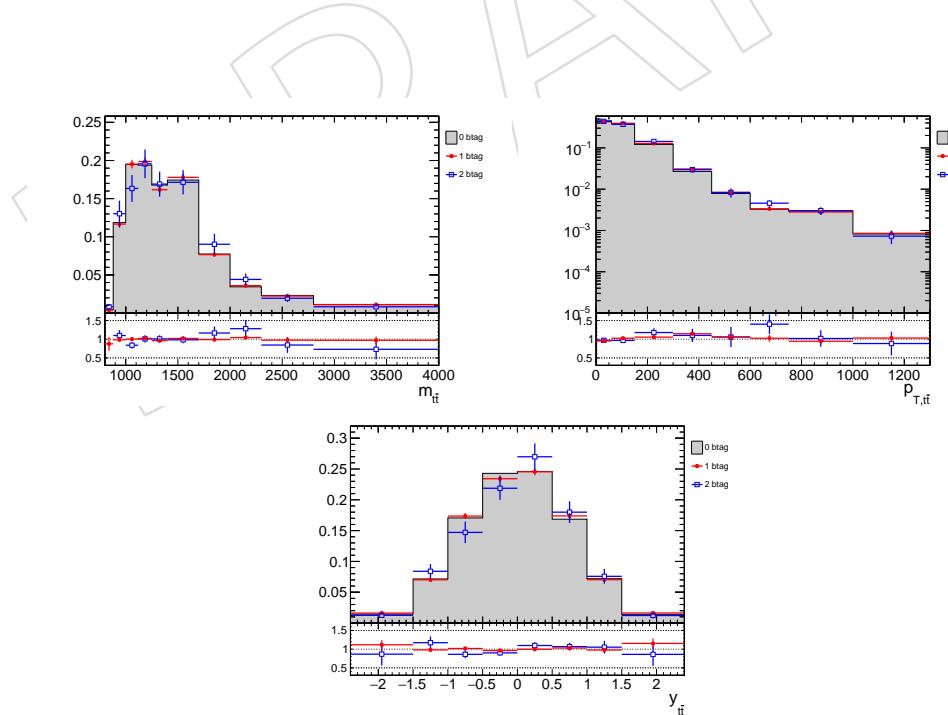


Figure 17: Closure test for the data-driven QCD prediction method for the shape of the $t\bar{t}$ variables.

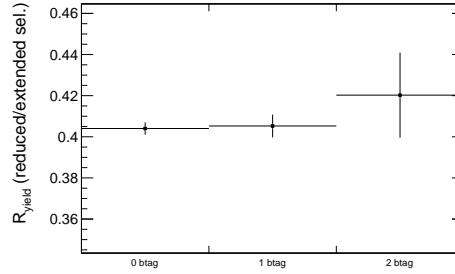


Figure 18: Closure test for the data-driven QCD prediction method for event yield ratio between the control and signal regions.

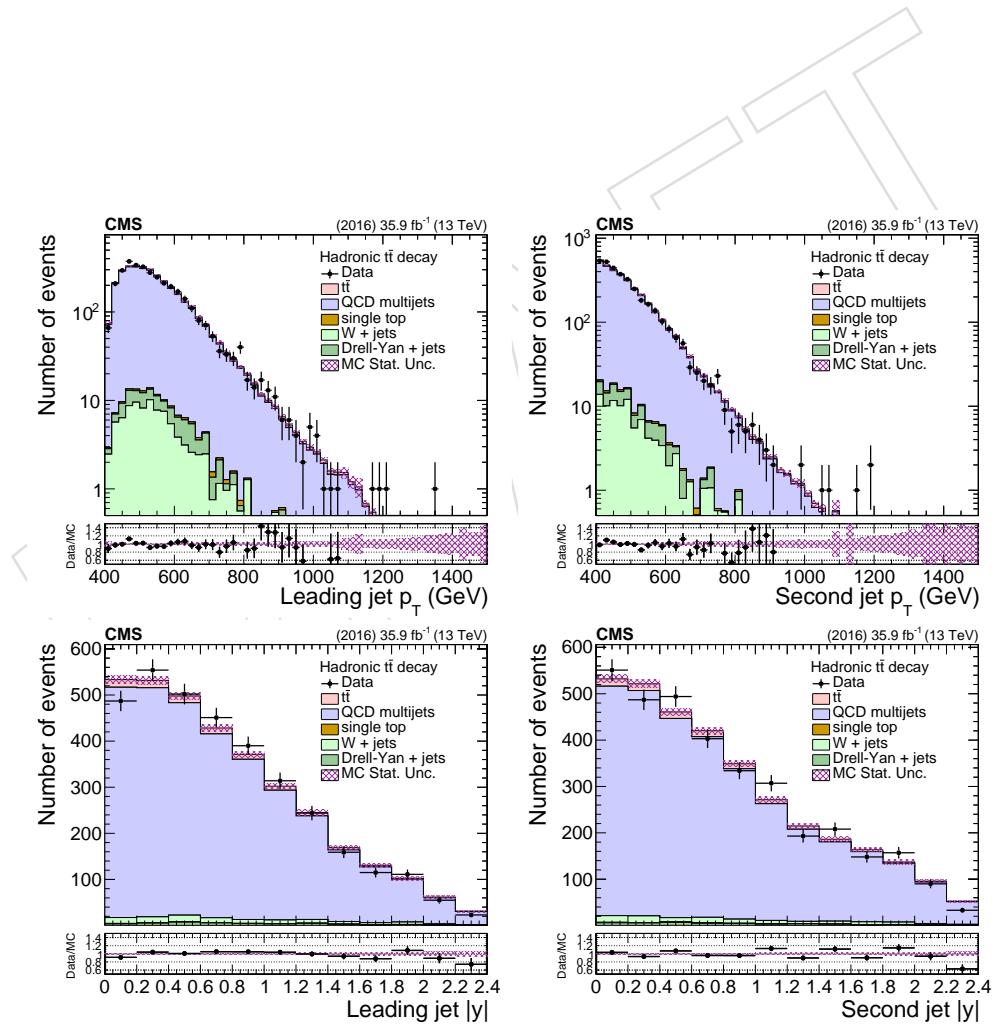


Figure 19: Jet p_T and $|y|$ distributions in the QCD control region.

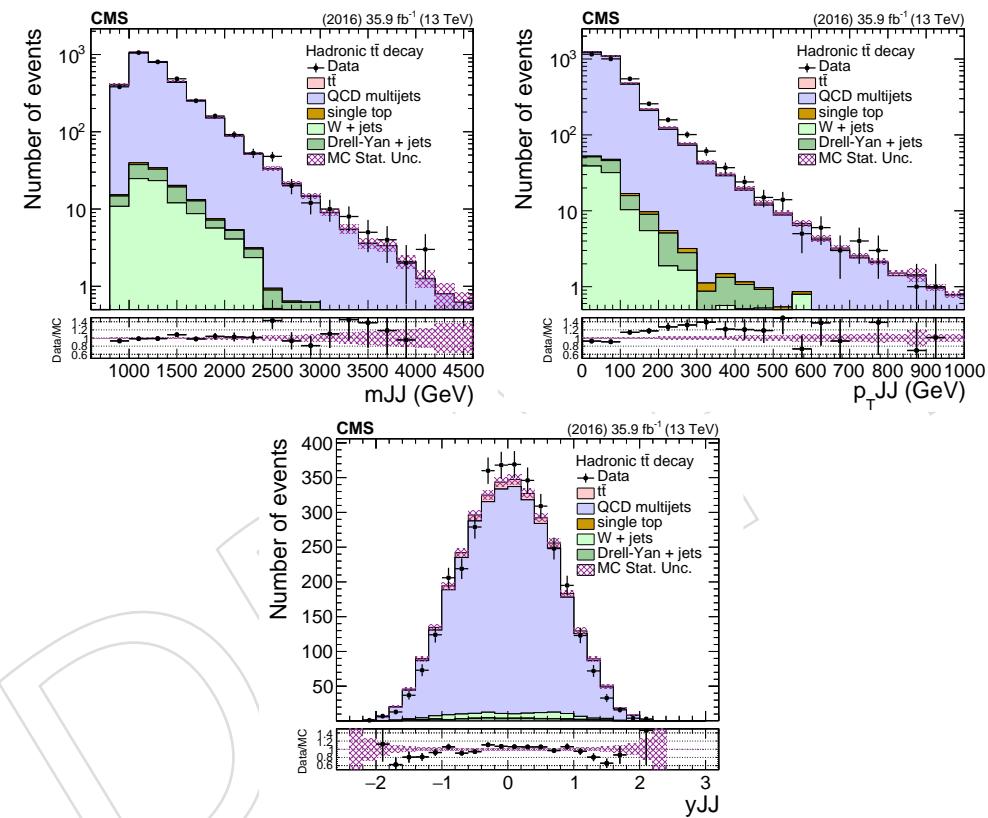


Figure 20: Kinematic distributions of the $t\bar{t}$ system in the QCD control region.

285 6 Data vs Monte Carlo

286 In this section we present comparisons between data and Monte Carlo for various observables.
 287 It should be noted that the $t\bar{t}$ normalization is scaled by a factor 0.635, consistent with the
 288 findings of Section 5, and the QCD background yield is adjusted such that the total Monte Carlo
 289 events are equal to the events in data. Table 9 shows the event yields for the various processes
 290 after applying the baseline selection plus the requirement that both AK8 jets contain a b-tagged
 291 subjet, with or without the NN cut (see Section 4 for details on the selection requirements).
 292 Already after the b-tagging requirement the $t\bar{t}$ signal is sufficiently enhanced that it becomes
 293 visible. Finally, the NN cut suppresses QCD by a factor ~ 17 with a signal loss of $\approx 45\%$. In
 294 the signal region the signal-over-background ratio is ≈ 1.8 .

Table 9: Expected and observed event yields in SR_A .

Process	No NN cut	With NN cut
$t\bar{t}$	10881	5867
QCD	85155	4930
W+jets	857	110
Z+jets	784	59
Single Top	753	211
Data	98430	11177

Table 10: Expected and observed event yields in the signal region.

Process	Yield
$t\bar{t}$	3978
QCD	2171
W+jets	51
Z+jets	12
Single Top	83
Data	6295

295 Figure 21 shows the softDrop mass of the leading jet, which serves as a proxy for the top
 296 mass. This is defined as the leading AK4 subjet in the leading AK8 jet and it is selected if
 297 the event satisfies the signal region selection and if it has $p_T > 300 \text{ GeV}$ while it is not b-tagged
 298 ($\text{CSV} < 0.8484$). The distribution of the NN output is shown in Fig. 22.
 299 The kinematic properties of jets in the signal region are shown in Figs. 23, 24, while those of the
 300 $t\bar{t}$ system are shown in Fig. 25. Finally, the jet substructure properties (n-subjettiness variables)
 301 are shown in Figs. 26, 27.

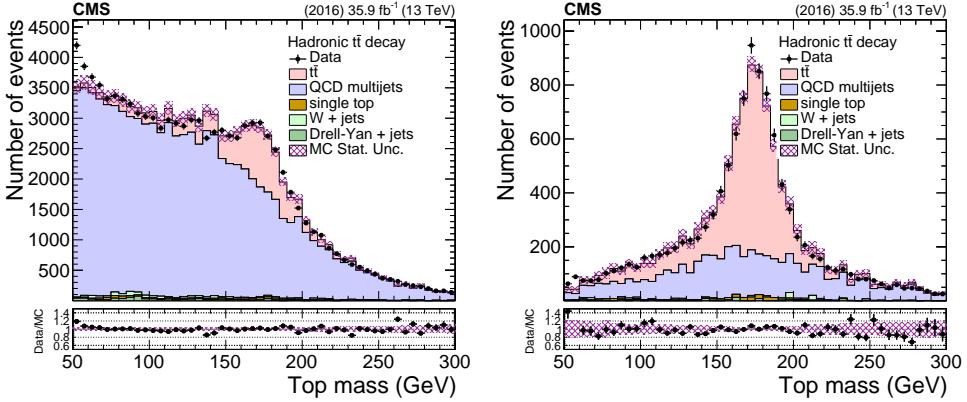


Figure 21: SoftDrop mass of the leading AK8 jet after the baseline selection with both AK8 jets containing a b-tagged subjets, with (right) and without (left) the $NN > 0.8$ cut.

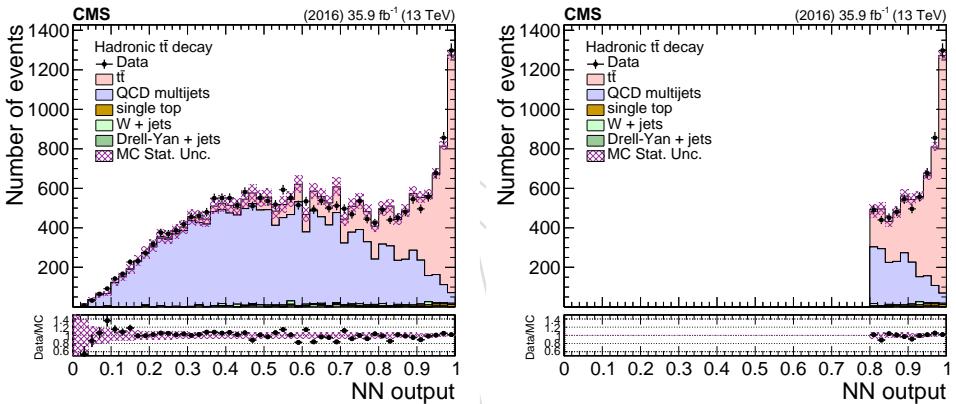


Figure 22: NN output after the baseline selection with both AK8 jets containing a b-tagged subjets, with (right) and without (left) the $NN > 0.8$ cut.

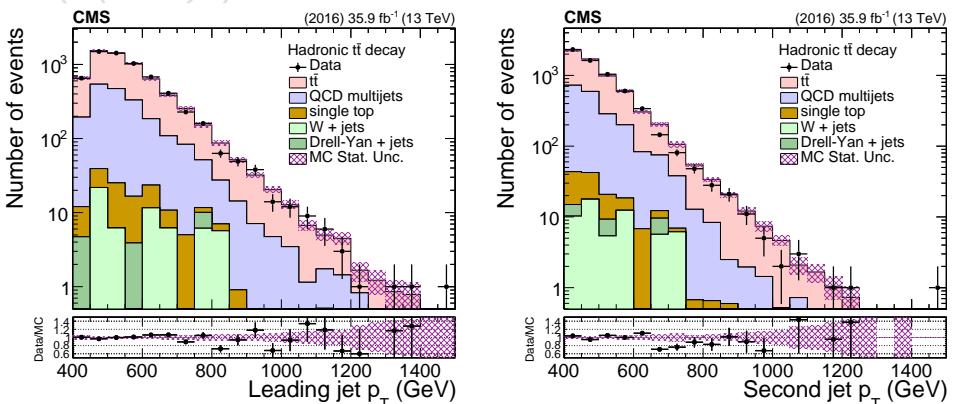


Figure 23: Distributions of the leading and second jet p_T in the signal region.

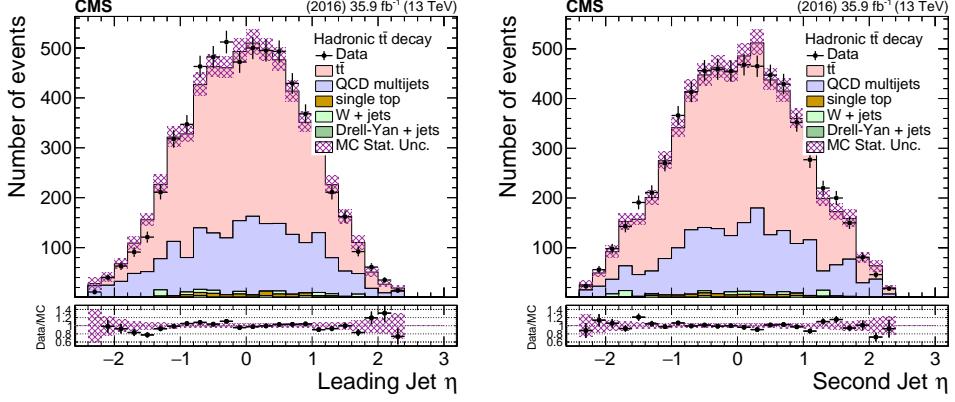


Figure 24: Distributions of the leading and second jet η in the signal region.

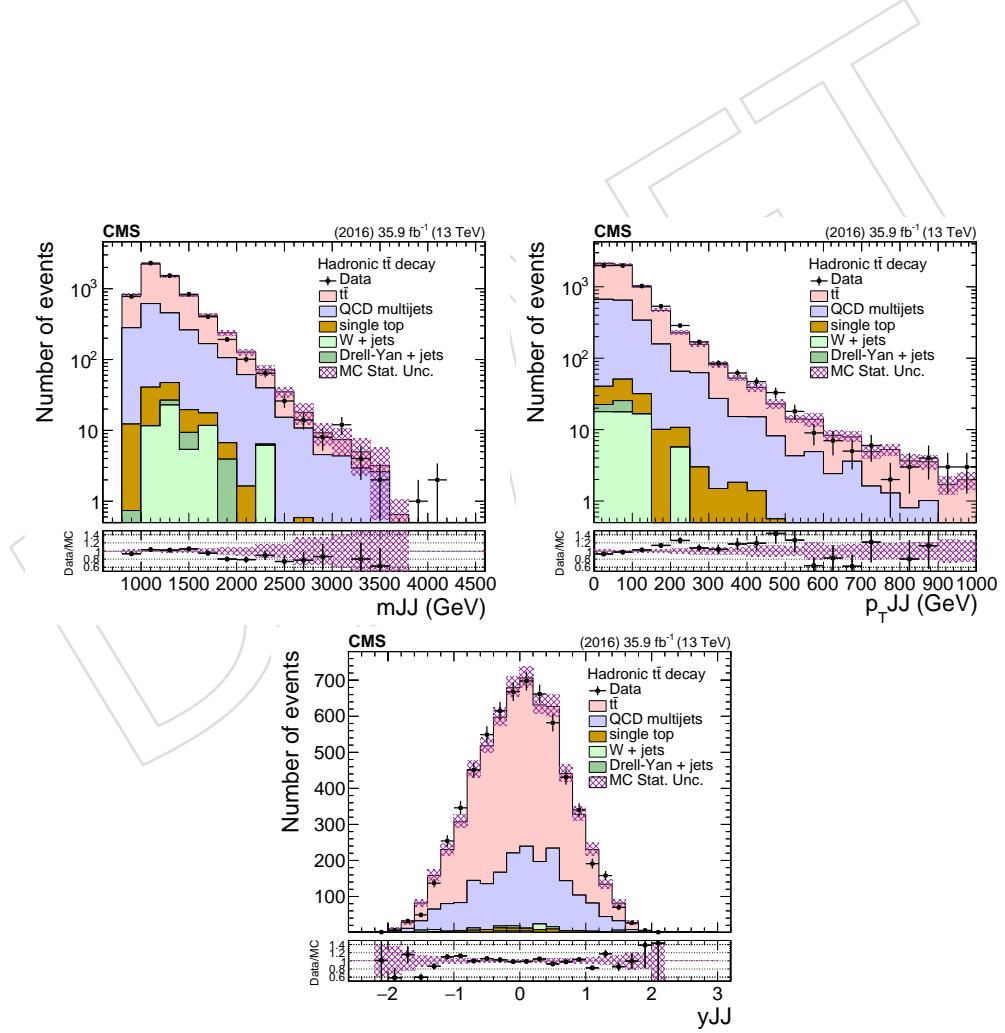


Figure 25: Kinematic distributions of the $t\bar{t}$ system in the signal region.

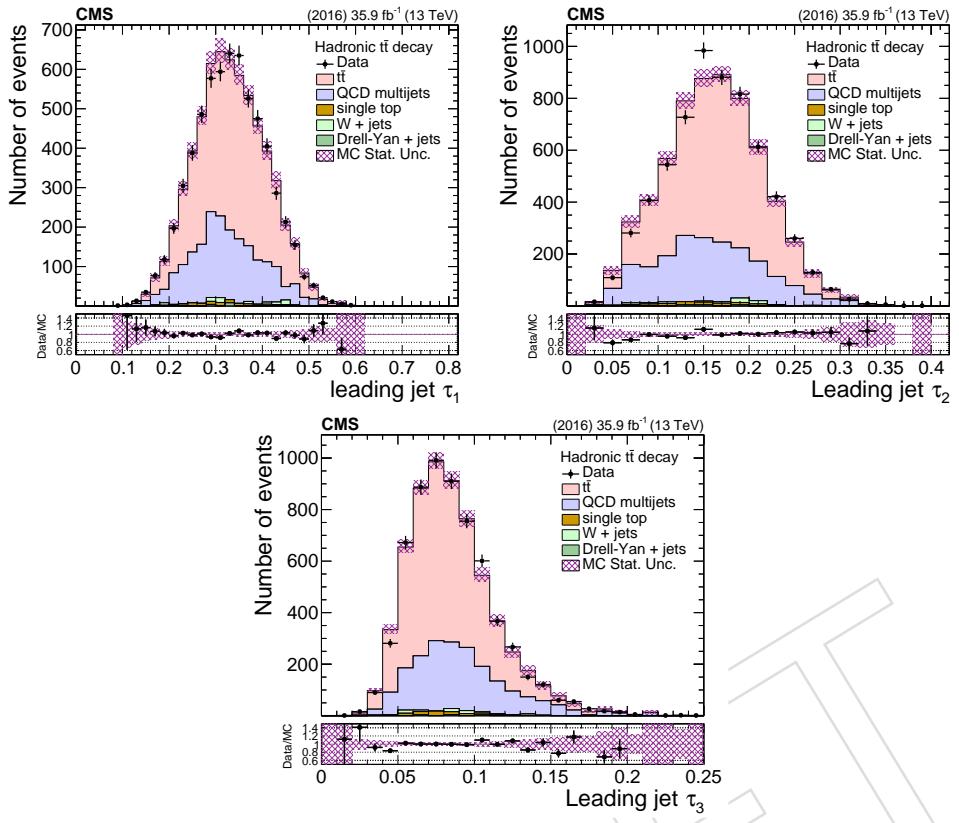


Figure 26: N-subjettiness variables for the leading jet in the signal region.

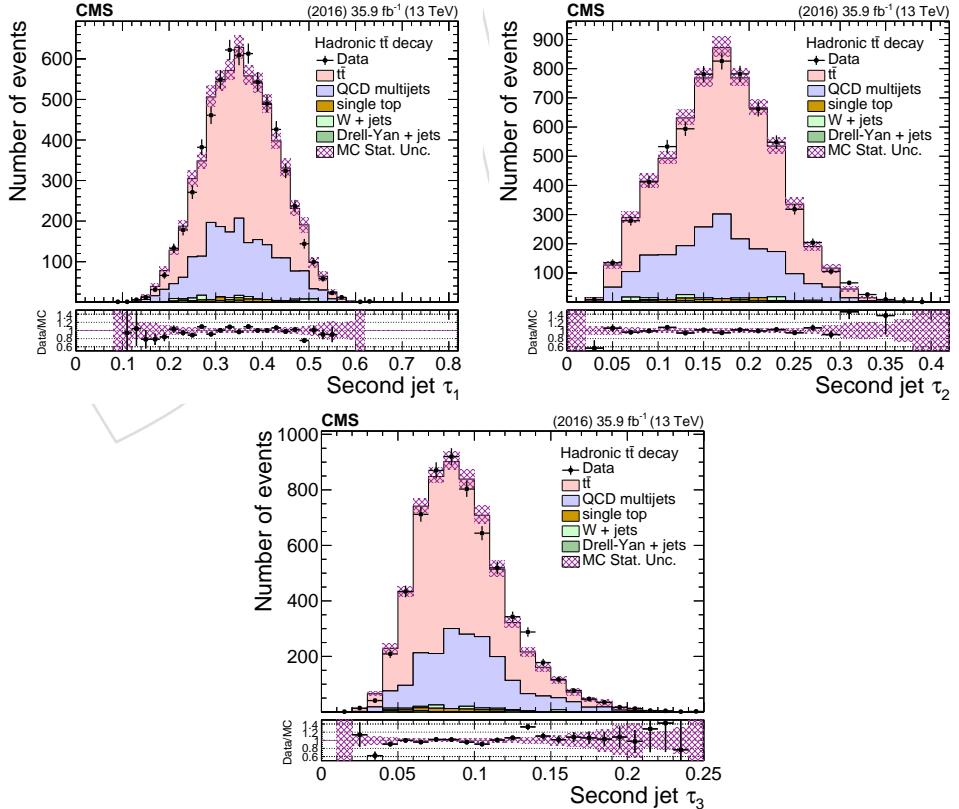


Figure 27: N-subjettiness variables for the second jet in the signal region.

302 7 Systematic Uncertainties

303 The systematic uncertainties considered in this analysis are divided in two categories: experimental and theoretical. The former includes all the uncertainties related to the differences in
 304 the object performance between data and simulation. The latter are related to the simulation it-
 305 self and affect primarily the unfolded results through the acceptance, efficiency, and migration
 306 matrix. The list below describes briefly these uncertainties and the way they have been han-
 307 dled here. It should be noted that for each systematic variation the differential cross sections
 308 (fiducial and unfolded) are re-measured and the difference with respect to the nominal result
 309 is taken as the effect of this variation to the measurement.

311 1. Experimental Uncertainties

- 312 • QCD background prediction: we use the fitted QCD yield uncertainty. The
 313 shape uncertainties due to the closure test in the simulation and the different
 314 pileup profiles in the control and signal regions are very small, at the 1% level.
- 315 • *Jet energy scale (JES)*: this is the uncertainty on the energy scale of each recon-
 316 structed jet and it is a leading experimental uncertainty. Following the rec-
 317 commendations of the JME group, we have considered 24 independent JES
 318 sources [41] as follows: for each variation a new jet collection is created and
 319 the event interpretation is repeated. This results not only in variations of the
 320 p_T scale itself, but may also lead to different top candidates. The JES uncer-
 321 tainty, per jet, is of the order 1 – 2%, p_T and η dependent. The effect on the
 322 measured cross section is typically of the order 10% but it can be much larger
 323 at very high jet p_T .
- 324 • *Jet energy resolution*: The impact on the measurement due to the jet energy res-
 325 olution (JER) is determined by smearing the jets according to the JER uncer-
 326 tainty. The effect on the cross section is relatively small, at the level of 2%.
- 327 • *Subjet b tagging efficiency (hadronic)*: The uncertainty in the identification of b-
 328 subjets within the large- R jets (estimated in [42]) is a leading experimental
 329 uncertainty in the hadronic channel. The effect on the cross sections is of the
 330 order of 10% relatively flat in all the observables. Unlike the uncertainty asso-
 331 ciated with the JES, the b-subjet tagging uncertainty therefore largely cancels
 332 in the normalized cross sections.
- 333 • *Pileup*: The uncertainty related to the modeling of additional pileup interac-
 334 tions is a subdominant uncertainty. The impact on the measurement is esti-
 335 mated by varying the total inelastic cross section used to weight the simulated
 336 events (69.2 mb) by $\pm 4.6\%$ [43]. The effect on the cross sections is negligible
 337 (below 1%).
- 338 • Trigger: this accounts for the difference between the simulated and observed
 339 trigger efficiency. Based on Fig. 2 the uncertainty is well below 1% in the phase
 340 space of this analysis.
- 341 • *Luminosity*: The uncertainty in the measurement of the integrated luminosity
 342 is 2.5% [44].

343 2. Theoretical Uncertainties

344 The theoretical uncertainties are divided into two sub-categories: the ones related to the
 345 matrix element of the hard process and the ones related to the modelling of the parton
 346 shower and the underlying event. Practically, the first category (consisting of the first

347 three sources below) is evaluated by variations of LHE event weights stored in the nominal
 348 MC simulation, while the second category is evaluated with dedicated, alternative
 349 MC samples.

- 350 • **Parton distribution functions:** The uncertainty due to parton distribution functions (PDFs) is estimated by applying event weights corresponding to the 100
 351 replicas of the NNPDF set [31]. For each observable we compute its standard
 352 deviation from the 100 variations.
- 353 • **Renormalization and factorization scales:** The uncertainty in the choice of renormalization and factorization scale is assessed by separately varying the renormalization and factorization scales by a factor of [2.0,0.5]. The unphysical anticorrelated variations are discarded, yielding a total of 7 combinations of the renormalization and factorization scales. The event weight is determined for each variation and the envelope is taken as the scale uncertainty, according to the prescription in [<https://indico.cern.ch/event/459797/contributions/1961581/attachments/1181555/1800214/mcaod-Feb15-2016.pdf>]. These variations are applied using the event weights provided in the LHEEventInfo [<https://twiki.cern.ch/twiki/bin/viewauth/CMS/LHEReaderCMSSW>].
- 354 • **Strong coupling constant (α_S):** The uncertainty associated with the α_S is estimated by applying event weights corresponding to higher and lower values
 355 of α_S for the matrix element using the variations of the NNPDF set [31].
- 356 • **Final state radiation (FSR):** this uncertainty is estimated from alternative MC
 357 samples with reduced and increased value for the strong coupling constant used by Pythia8 to generate final state radiation (α_S^{FSR} by factors $\sqrt{2}$ and $1/\sqrt{2}$). However, the default variations are largely exaggerated, as seen in Fig. 28,
 358 where the alternative samples fail miserably to describe the data in two sensitive observables: the mass of the top candidate jet and the NN output, both of which rely on the dynamics of the jet formation. In order to use a more realistic estimate of this uncertainty, a maximum likelihood fit is performed (independently) on these variables, using the systematic uncertainties as independent
 359 nuisance parameters. The fits are implemented through the "Combine" tool-
 360 box using templates for the various components and are shown in Fig. 29. The fit on the m_t variable is well behaved in the entire fit range, while the fit on the
 361 NN output is less successful in the background-enriched region. Nevertheless,
 362 since it is the signal uncertainties that we wish to constrain, the signal region is
 363 fitted perfectly. As a result of these fits, the nuisances are constrained in-situ.
 364 Figures 30 and 31 show the comparison of the pre-fit and post-fit uncertainties,
 365 as well as the pulls of the nuisance parameters. Both fits indicate that the post-
 366 fit FSR nuisance is actually close to its pre-fit (nominal) value with a significant
 367 reduction of its uncertainty. Based on the observations from the fits, we have
 368 scaled down the effects of the FSR variations by a (conservative) factor 0.3.
- 369 • **Initial state radiation (ISR):** this uncertainty is estimated from alternative MC
 370 samples with reduced and increased value for the strong coupling constant used by Pythia8 to generate initial state radiation (α_S^{ISR} scaled by factors of 2 and 0.5).
- 371 • **Matrix element – parton shower matching:** In the POWHEG matrix element to parton shower (ME-PS) matching scheme, the resummation damping factor h_{damp} is used to regulate high- p_T radiation. Uncertainties in h_{damp} are parameterized by considering alternative simulated samples with h_{damp} varied by $h_{damp} = m_t$ and $h_{damp} = 2.24m_t$.

- 395 • *Underlying event tune:* This uncertainty is estimated from alternative Monte
 396 Carlo samples with the tune CUETP8M2T4 parameters varied by $\pm 1\sigma$.

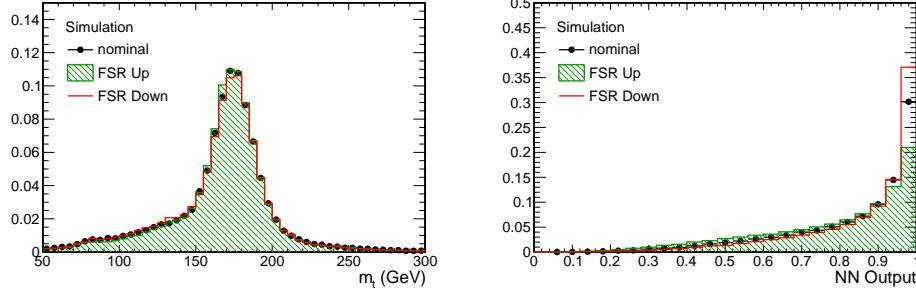


Figure 28: Variations of the m^t (left) and NN output (right) distributions due to the alternative FSR MC samples.

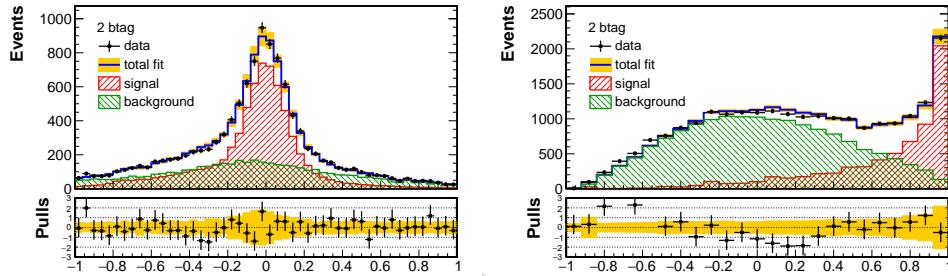


Figure 29: Fit to the m^t (left) and NN output (right) distributions aiming to constrain the MC modelling uncertainties.

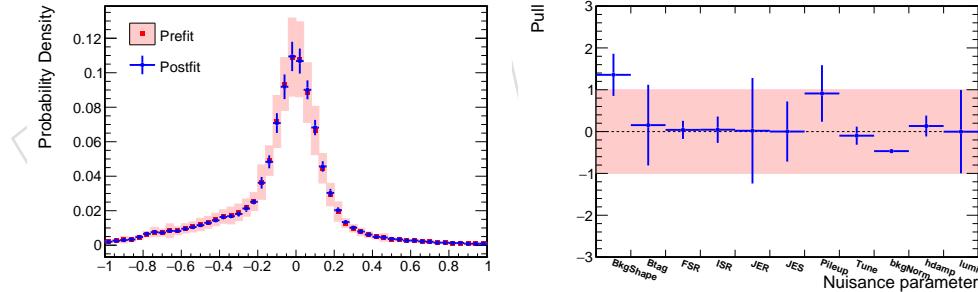


Figure 30: (left) Comparison between the prefit and postfit distributions and uncertainties of the m^t distribution. (right) Fit pulls of the nuisance parameters.

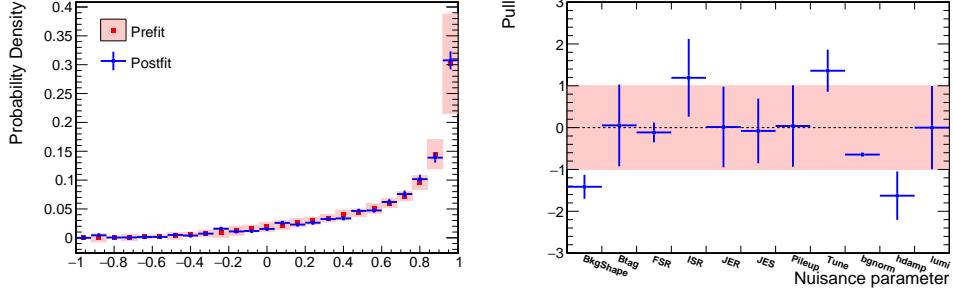


Figure 31: (left) Comparison between the prefit and postfit distributions and uncertainties of the NN output distribution. (right) Fit pulls of the nuisance parameters.

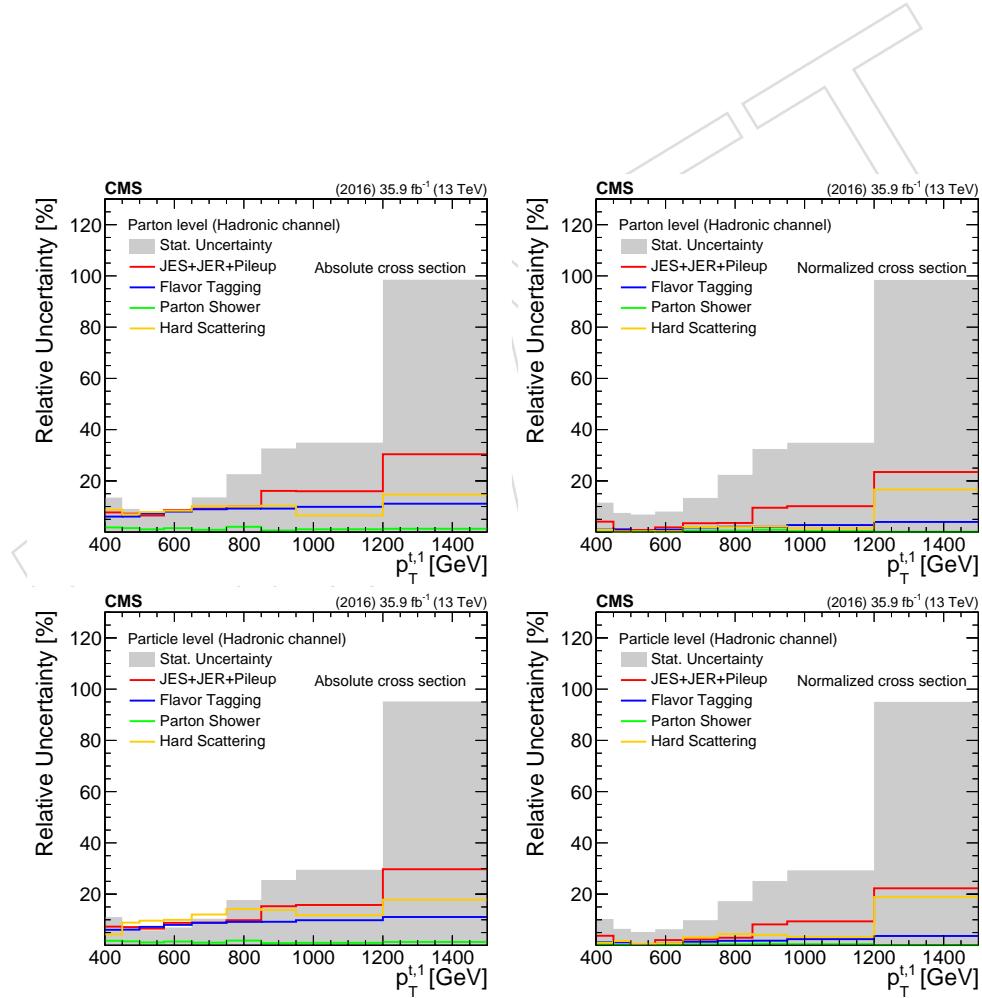


Figure 32: Decomposition of uncertainties for the parton- and particle-level measurement (left: absolute, right: normalized) as a function of the leading top p_T .

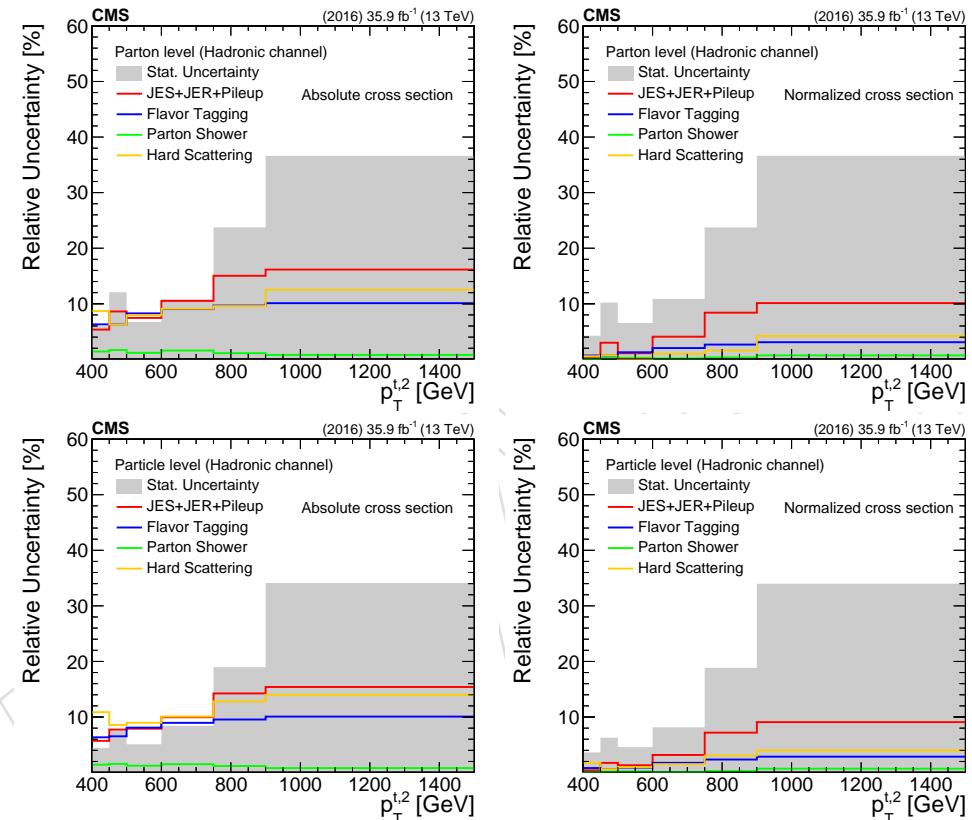


Figure 33: Decomposition of uncertainties for the parton- and particle-level measurement (left: absolute, right: normalized) as a function of the second top p_T .

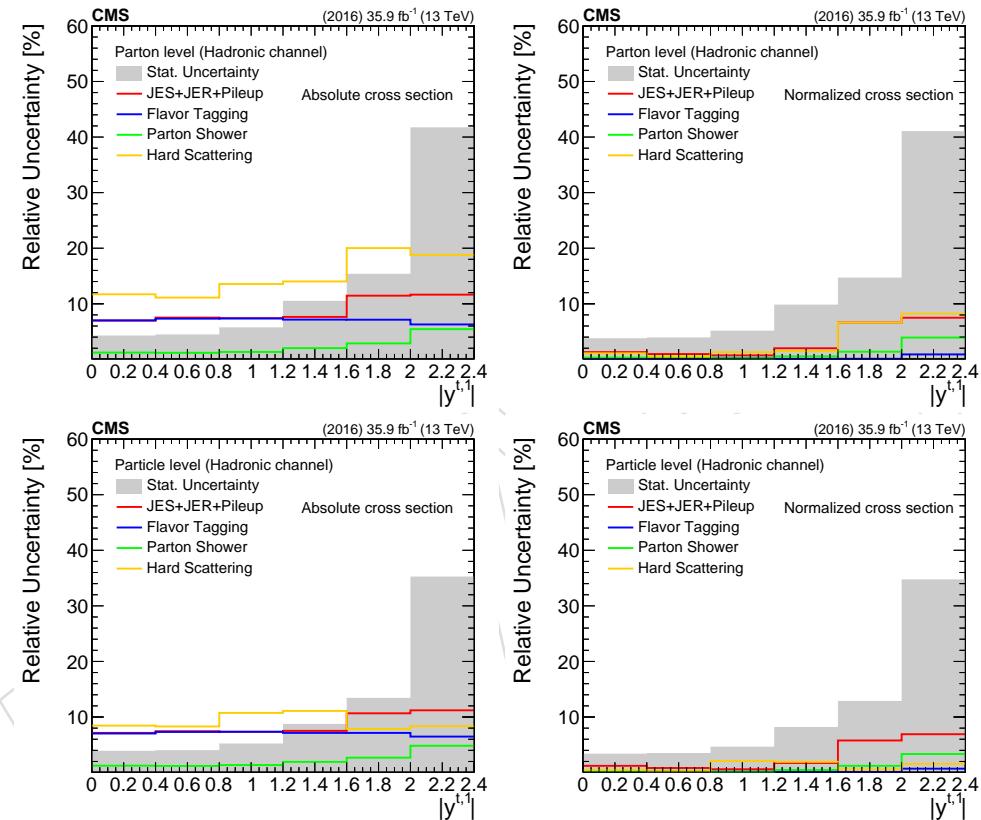


Figure 34: Decomposition of uncertainties for the parton- and particle-level measurement (left: absolute, right: normalized) as a function of the leading top $|y|$.

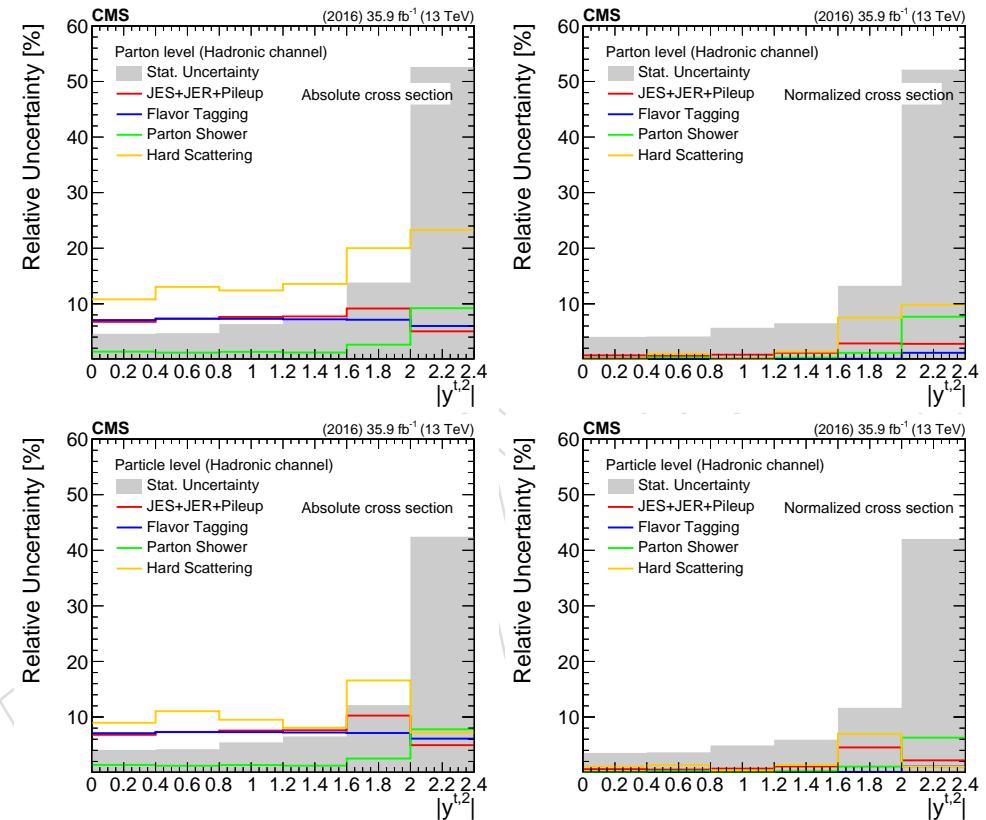


Figure 35: Decomposition of uncertainties for the parton- and particle-level measurement (left: absolute, right: normalized) as a function of the second top $|y|$.

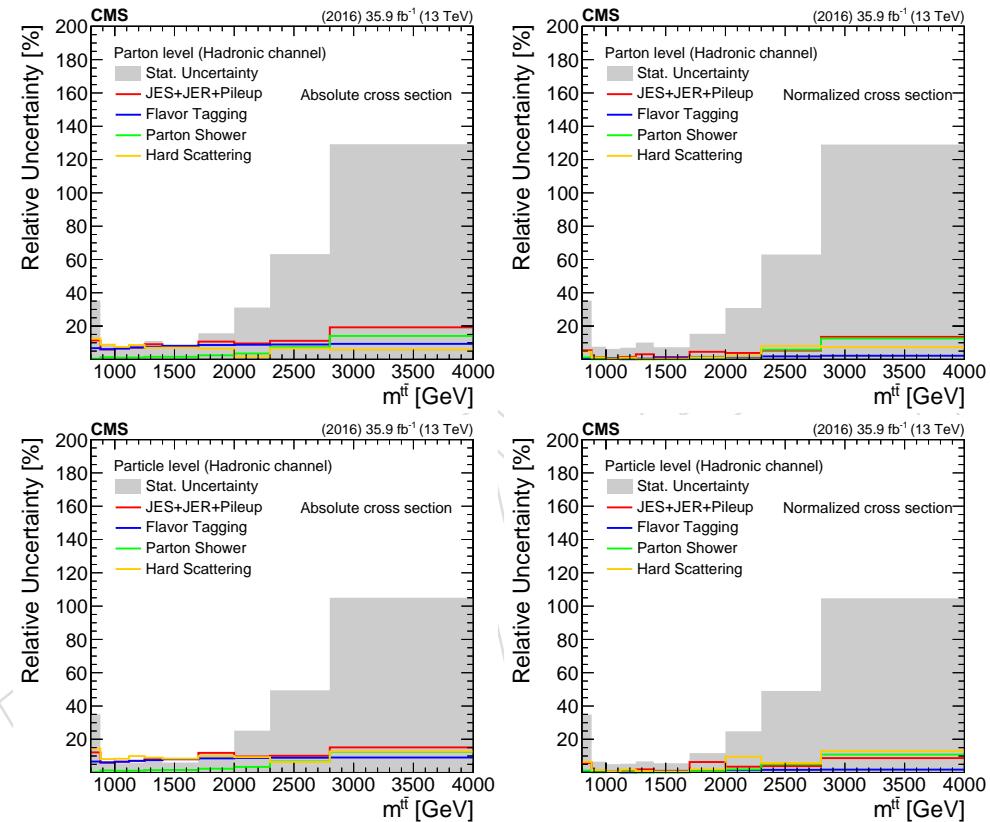


Figure 36: Decomposition of uncertainties for the parton- and particle-level measurement (left: absolute, right: normalized) as a function of $m_{\bar{t}\bar{t}}$.

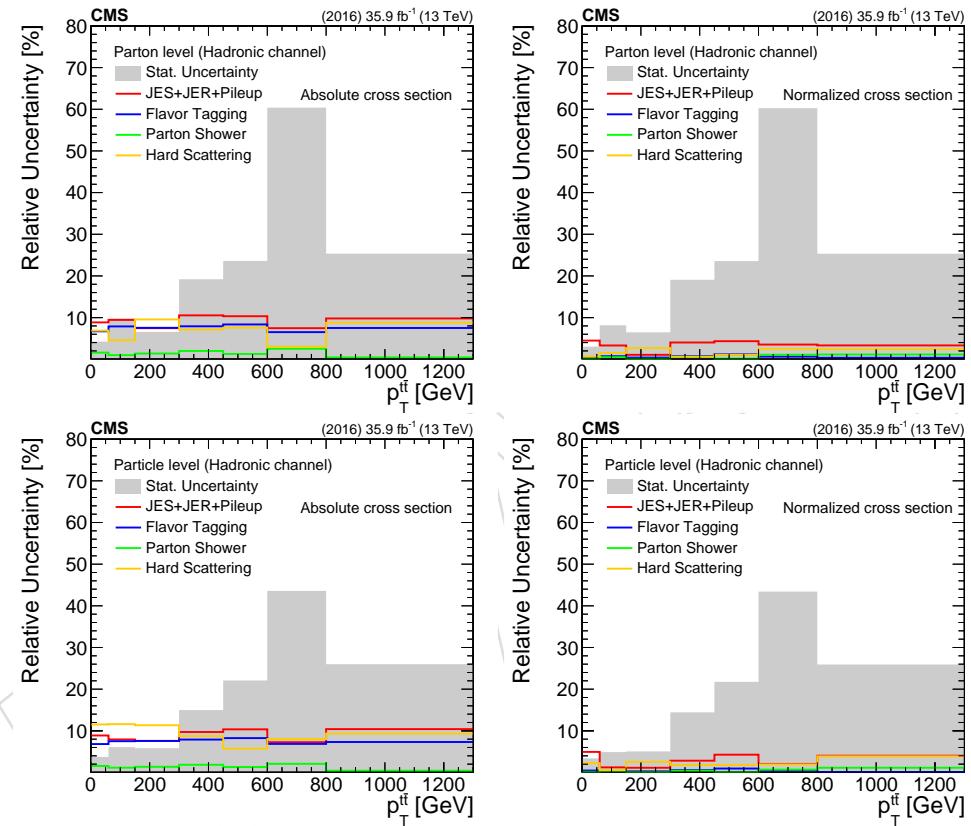


Figure 37: Decomposition of uncertainties for the parton- and particle-level measurement (left: absolute, right: normalized) as a function of p_T^t .

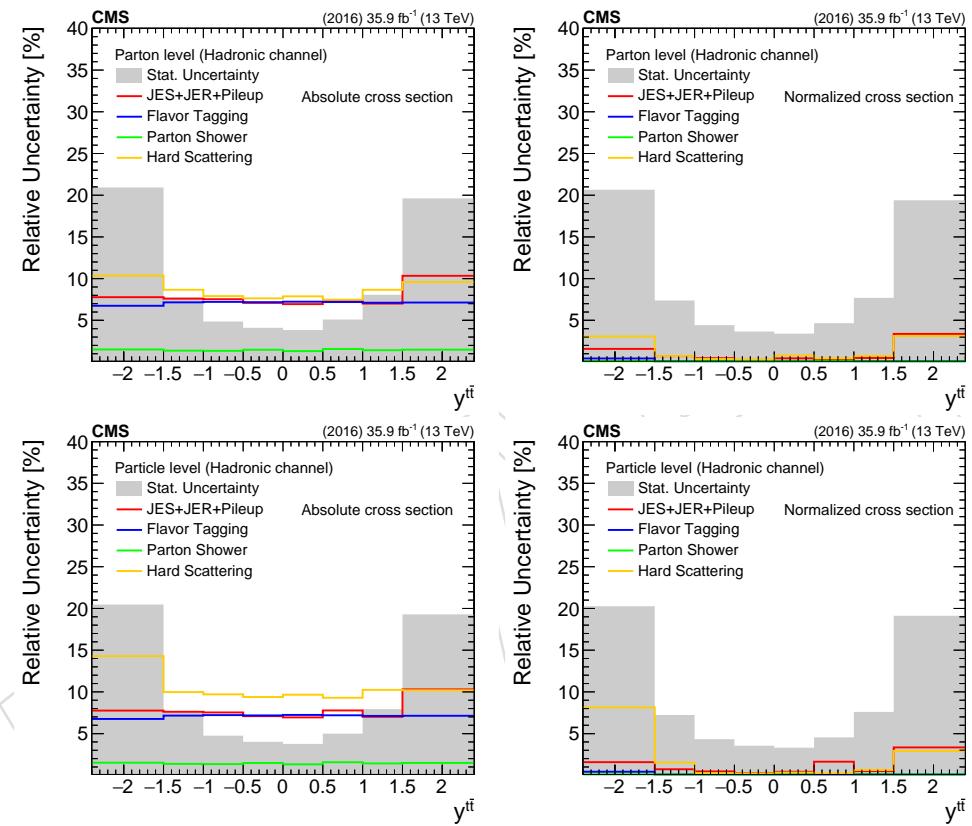


Figure 38: Decomposition of uncertainties for the parton- and particle-level measurement (left: absolute, right: normalized) as a function of $y_{t\bar{t}}$.

397 8 Fiducial Measurement

398 The fiducial differential cross section is derived in bin i of the variable x from the signal yield
 399 S_i (eq. 3) in the bin as follows:

$$\frac{d\sigma_i^{\text{fid}}}{dx} = \frac{S_i}{\mathcal{L} \cdot \Delta x_i}, \quad (4)$$

400 where \mathcal{L} is the total integrated luminosity and Δx_i is the width of the i -th bin of the observable
 401 x . Of particular interest is also the normalized cross section, computed as:

$$\frac{1}{\sigma^{\text{fid}}} \frac{d\sigma_i^{\text{fid}}}{dx} = \frac{1}{\sum_k S_k} \cdot \frac{S_i}{\mathcal{L} \cdot \Delta x_i}, \quad (5)$$

402 which is used to confront the modelling of the differential cross section regardless of the overall
 403 normalization. In order to estimate the uncertainty on the measurement, the entire procedure is
 404 repeated for every source of uncertainty described in Section 7. Both the experimental and the
 405 theoretical uncertainties affect primarily the $t\bar{t}$ singal shape, which is used to fit the data for the
 406 QCD background normalization. As a result the total systematic uncertainty of the measure-
 407 ment is small and the statistical uncertainty dominates. This is true both for the absolute and
 408 the normalized cross sections. Figures 39-45 show the fiducial cross sections as a function of
 409 the variables of interest. Firstly, we observe the expected offset of about 35% in the total cross
 410 section between the data and the Powheg+Pythia8 prediction, which is considerably smaller
 411 for the other theory predictions. In particular the Powheg+Herwigpp seems to agree best (this
 412 is most visible in Fig. 41). In terms of shape comparisons, the Powheg+Pythia8 prediction is in
 413 excellent agreement with data for all the variables, except for the invariant mass $m_{t\bar{t}}$ of the $t\bar{t}$
 414 system, where the theoretical spectrum appears to be harder above ≈ 2 TeV. A similar behavior
 415 is observed for the other theory models with hints of somewhat larger differences, although the
 416 statistical precision of the predictions does not allow quantitative comparisons.

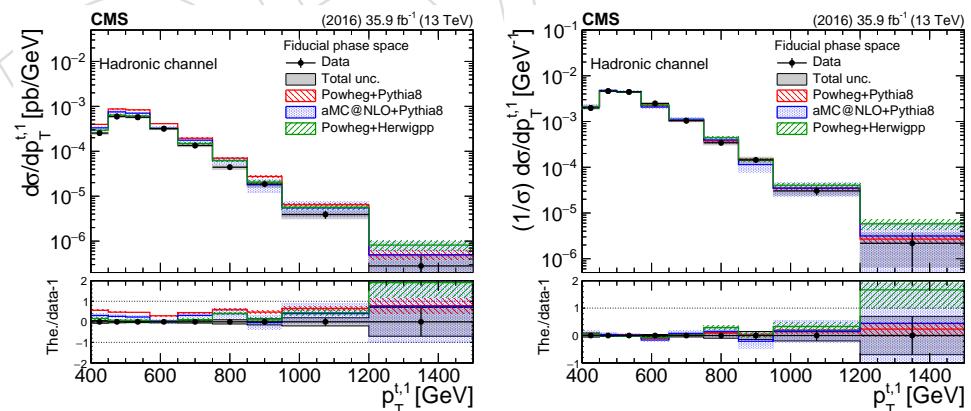


Figure 39: Fiducial differential cross section, absolute (left) and normalized (right), as a function of the leading top p_T . The bottom panel shows the ratio (theory - data)/data.

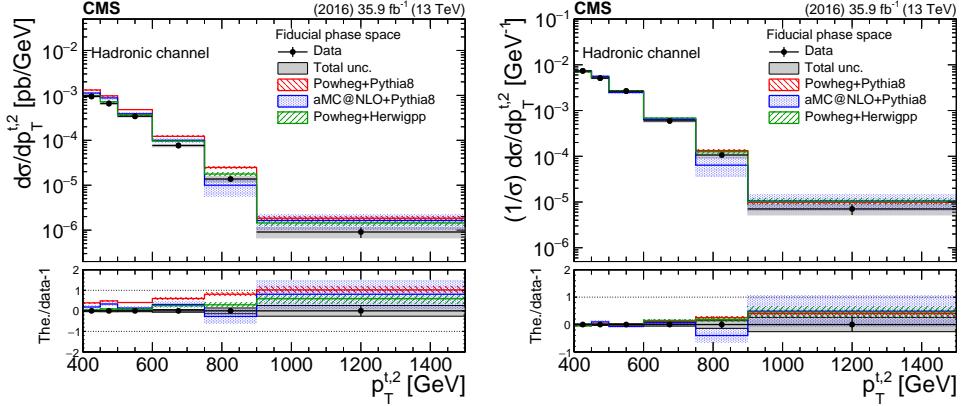


Figure 40: Fiducial differential cross section, absolute (left) and normalized (right), as a function of the second top p_T . The bottom panel shows the ratio (theory - data)/data.

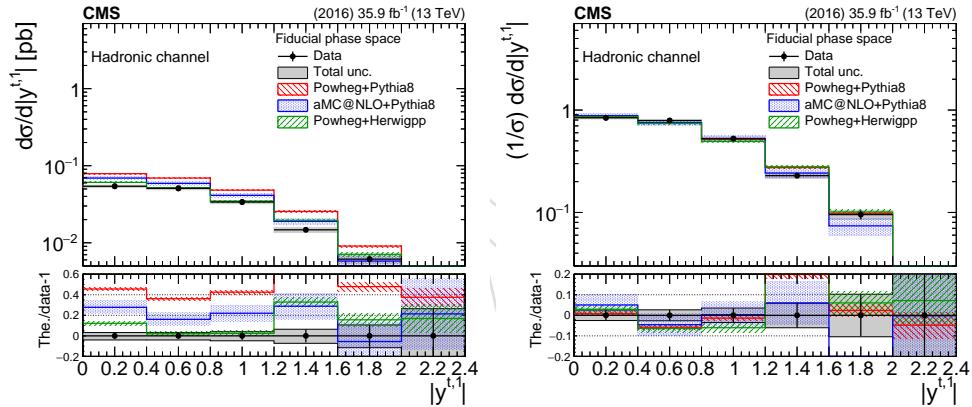


Figure 41: Fiducial differential cross section, absolute (left) and normalized (right), as a function of the leading top $|y|$. The bottom panel shows the ratio (theory - data)/data.

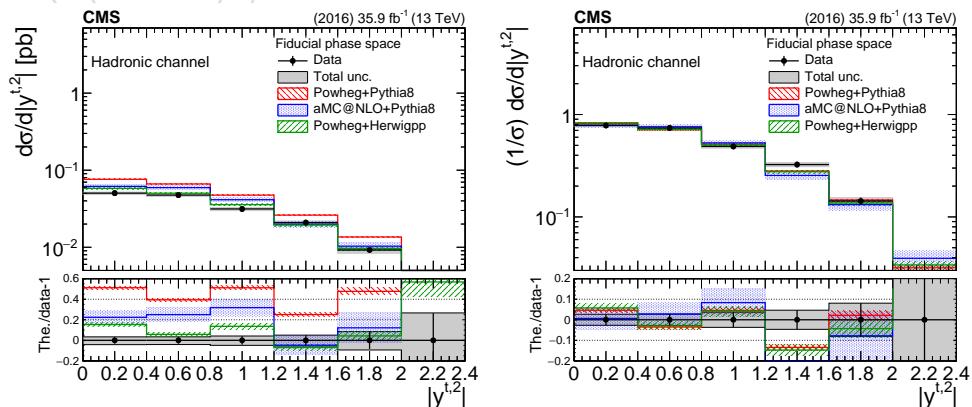


Figure 42: Fiducial differential cross section, absolute (left) and normalized (right), as a function of second top $|y|$. The bottom panel shows the ratio (theory - data)/data.

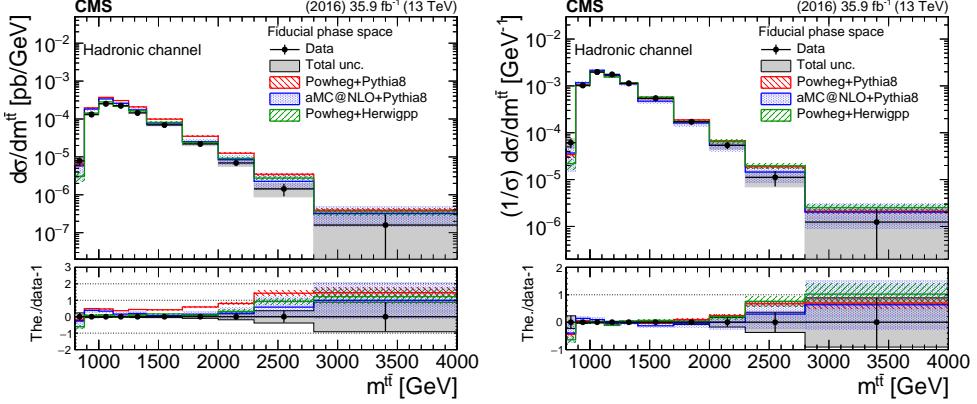


Figure 43: Fiducial differential cross section, absolute (left) and normalized (right), as a function of $m_{t\bar{t}}$. The bottom panel shows the ratio (theory - data)/data.

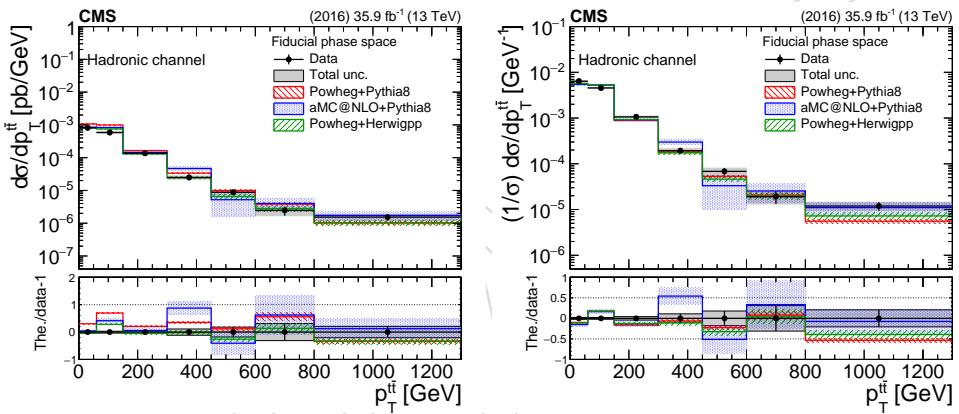


Figure 44: Fiducial differential cross section, absolute (left) and normalized (right), as a function of $p_T^{t\bar{t}}$. The bottom panel shows the ratio (theory - data)/data.

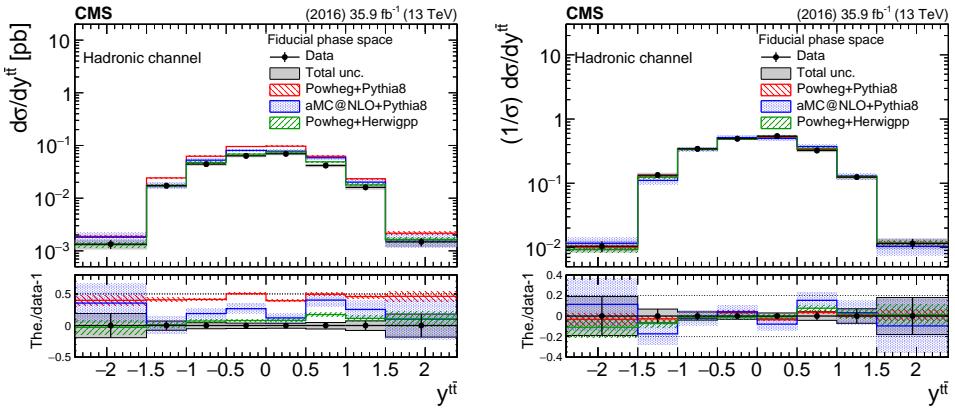


Figure 45: Fiducial differential cross section, absolute (left) and normalized (right), as a function of top $y_{t\bar{t}}$. The bottom panel shows the ratio (theory - data)/data.

417 9 Unfolded Measurement

418 The fiducial measurement at detector level is also reported unfolded to the parton and particle
 419 levels. Equation 6 defines the unfolded differential cross section:

$$\frac{d\sigma_i^{\text{unf}}}{dx} = \frac{1}{\mathcal{L} \cdot \Delta x_i} \cdot \frac{1}{f_{2,i}} \cdot \sum_j \left(R_{ij}^{-1} \cdot f_{1,j} \cdot S_j \right), \quad (6)$$

420 where \mathcal{L} is the total integrated luminosity and Δx_i is the width of the i-th bin of the observable
 421 x . The quantity $f_{1,j}$ is the fraction of reconstructed events in the j-th bin that have an equiva-
 422 lence event at the unfolded level (parton or particle), whereas the quantity $f_{2,i}$ is the fraction of
 423 events at the unfolded level that have an equivalent reconstructed event. Figures 46 and 57 be-
 424 low show the aforementioned fractions at parton and particle level, respectively, as a function
 425 of all the observables. The quantity R_{ij}^{-1} is the inverse of the migration matrix between the i-th
 426 and j-th bins. Due to the finite resolution of the detector, the migration matrix is non-diagonal
 427 and thus the application of an unfolding procedure is necessary. The binning of the various
 428 observables has been chosen such that the purity (fraction of reconstructed events that the true
 429 value of the observable lies in the same bin) and the stability (fraction of true events that the re-
 430 constructed observable lies in the same bin) are well above 50% (Figures 47 and 58). This choice
 431 results in highly diagonal migration matrices, shown in Figs. 48 and 59. In order to avoid the
 432 biases introduced by the various unfolding methods with some type of regularization, we have
 433 used simple migration matrix inversion, as written in Eq. 6 at a price of a moderate increase of
 434 the statistical uncertainty (see details in Appendix E).

435 9.1 Parton Level

436 The results of the unfolded measurement at parton level are shown in Figs. 49–55. The compari-
 437 son with the theory predictions follows the trends observed in the fiducial measurement. That
 438 is, there is a 20–40% lower inclusive cross section, while the shapes of the differential distri-
 439 butions are reasonably reproduced by all models. A hint of a deviation at very high values of
 440 $m^{t\bar{t}}$ is observed but the measurement is not very precise at this part of the phase space.

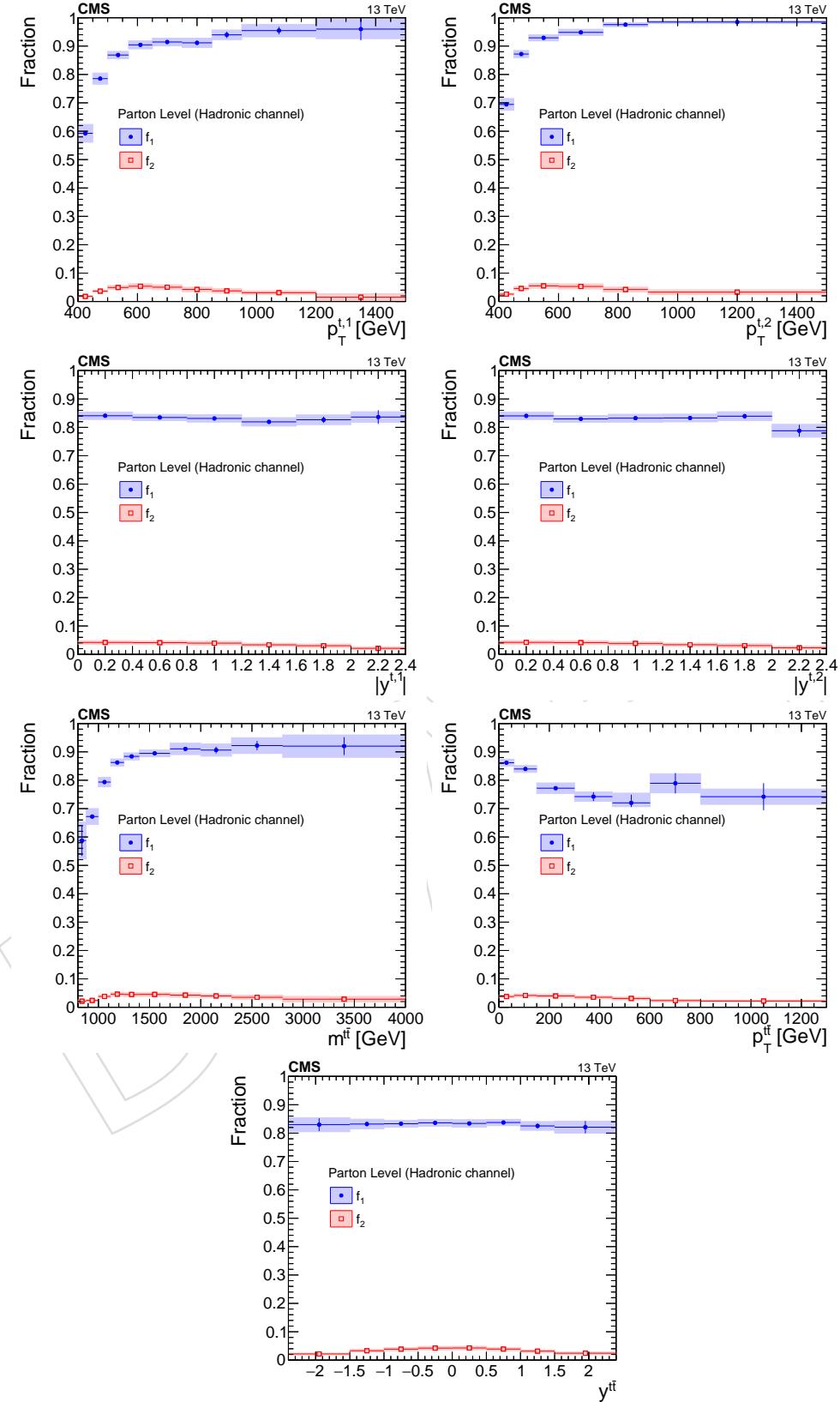


Figure 46: Simulated fractions $f_{1,2}$ for the parton-level selection as a function of the various observables.

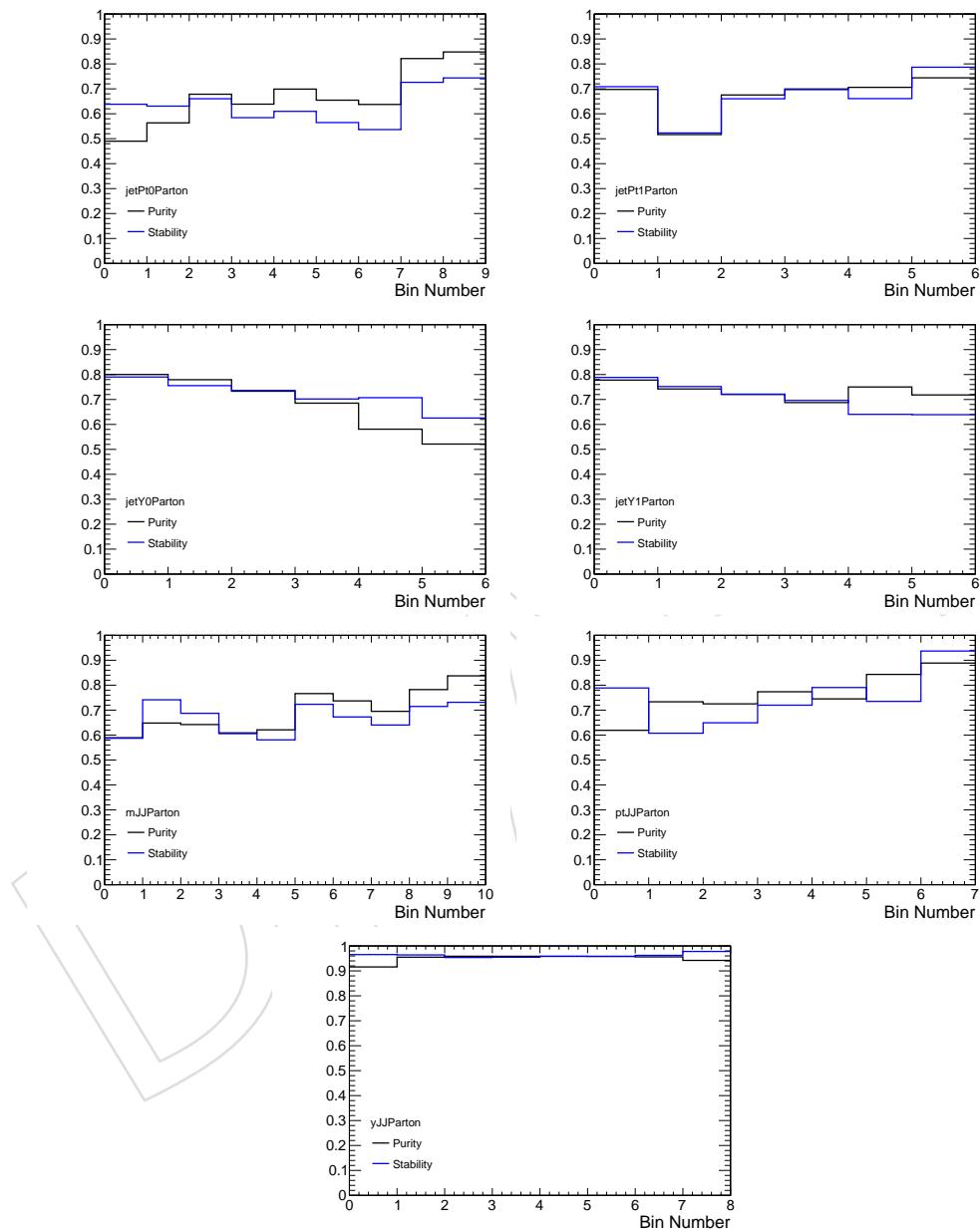


Figure 47: Simulated purity and stability of each bin at parton level.

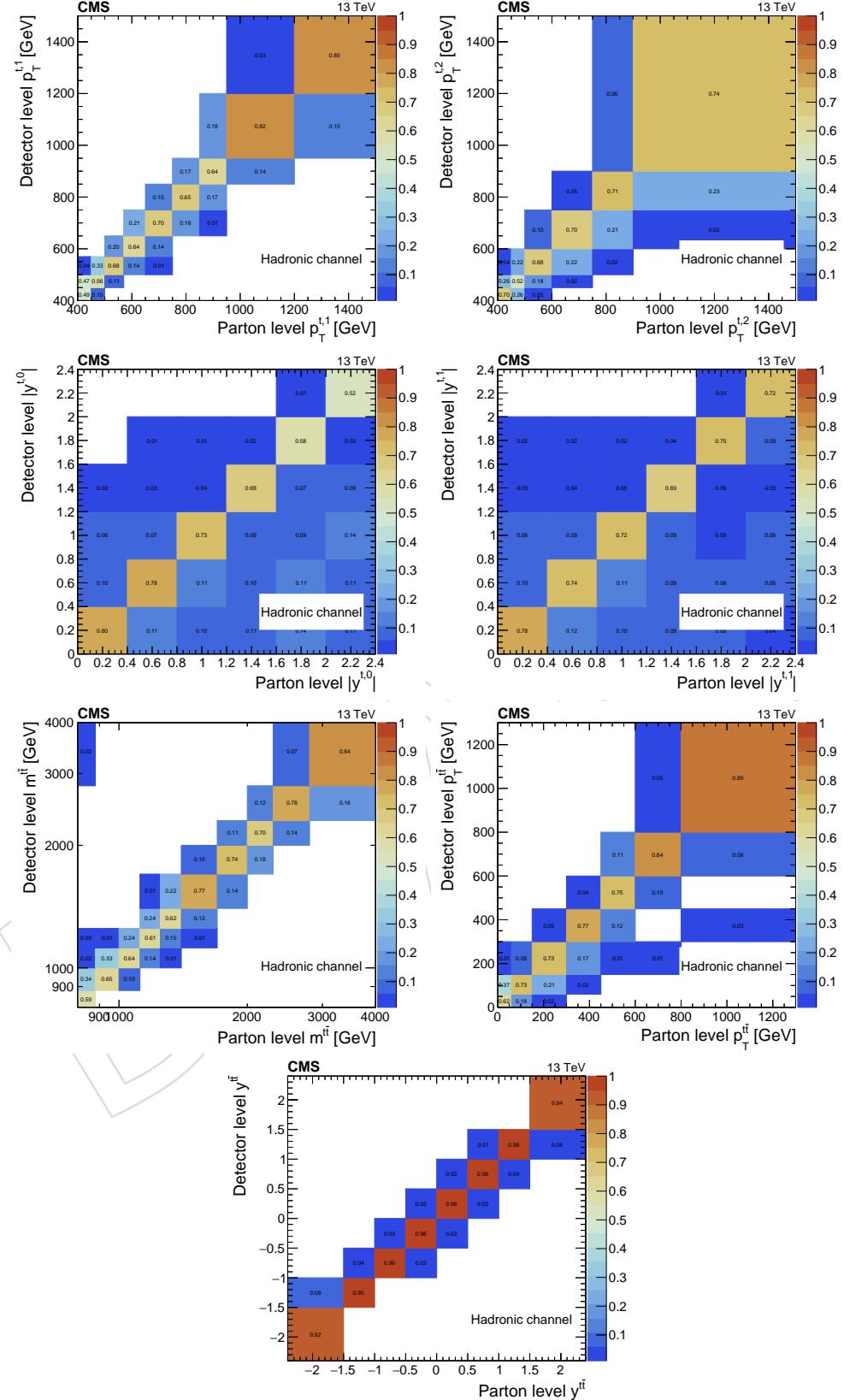


Figure 48: Simulated migration matrices at parton level. Each column is normalized to unity.

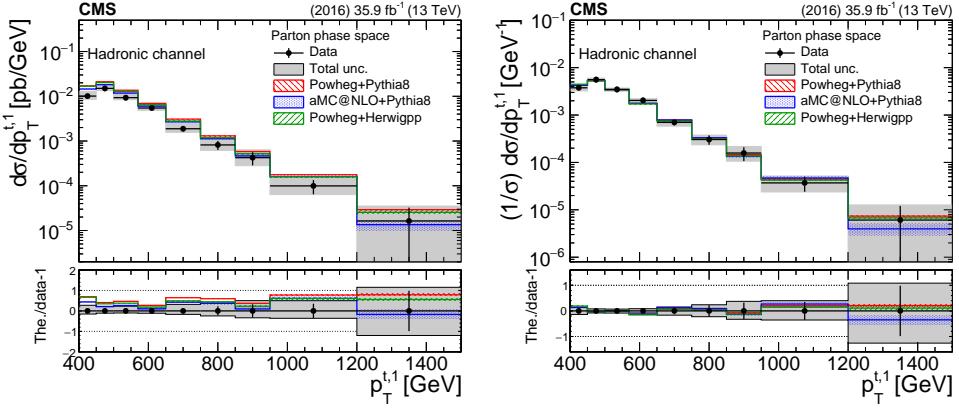


Figure 49: Differential cross section unfolded to parton level, absolute (left) and normalized (right), as a function of the leading top p_T . The bottom panel shows the ratio (theory - data)/data.

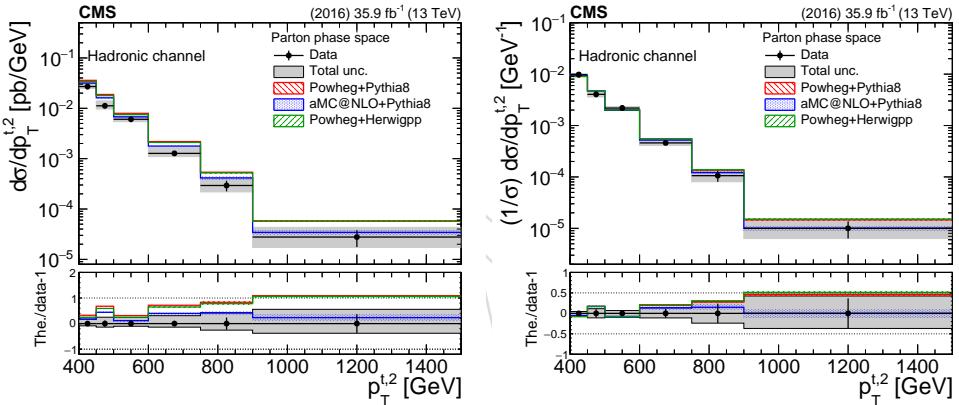


Figure 50: Differential cross section unfolded to parton level, absolute (left) and normalized (right), as a function of the second top p_T . The bottom panel shows the ratio (theory - data)/data.

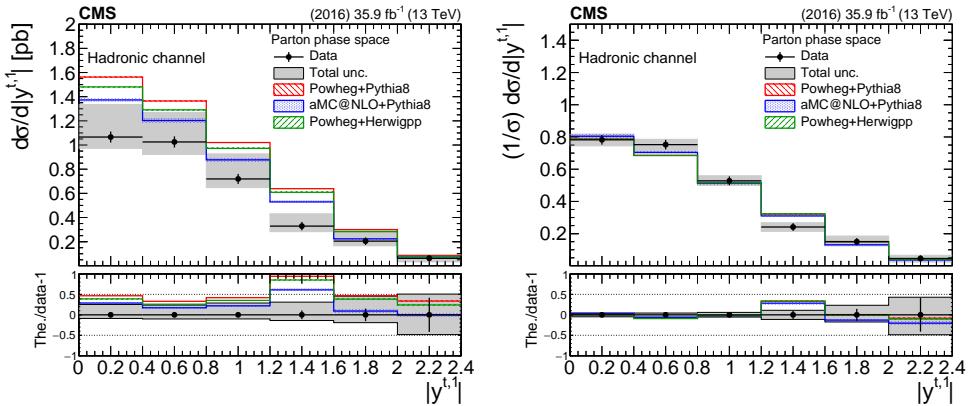


Figure 51: Differential cross section unfolded to parton level, absolute (left) and normalized (right), as a function of the leading top $|y|$. The bottom panel shows the ratio (theory - data)/data.

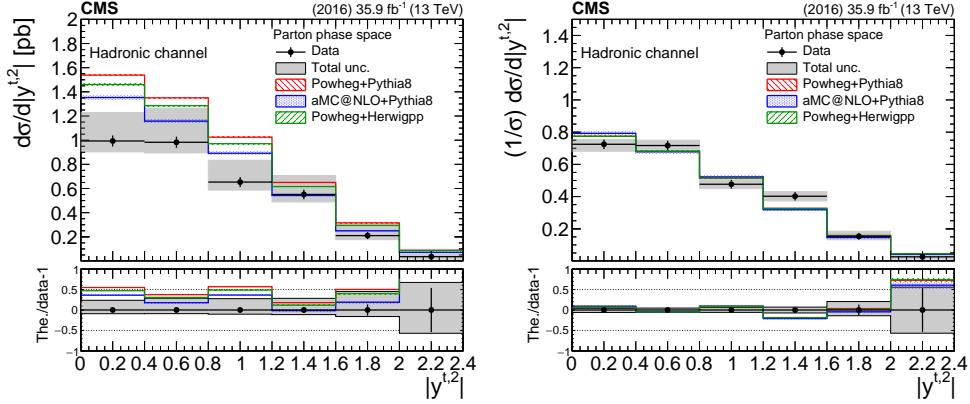


Figure 52: Differential cross section unfolded to parton level, absolute (left) and normalized (right), as a function of the second top $|y|$. The bottom panel shows the ratio (theory - data).

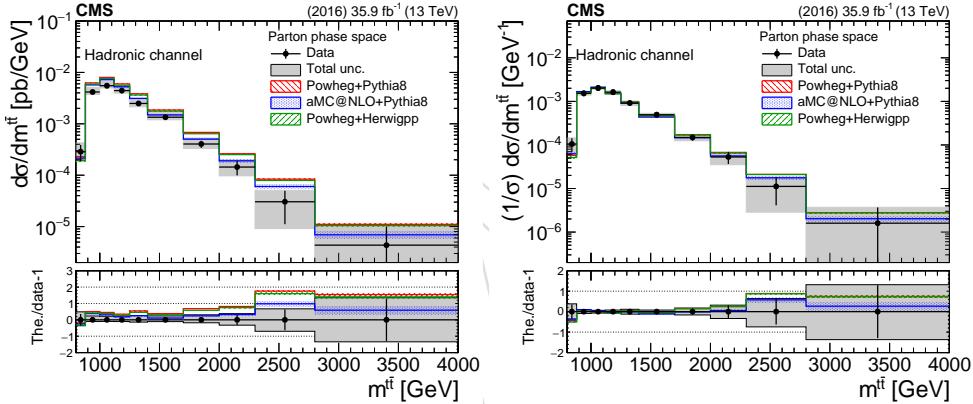


Figure 53: Differential cross section unfolded to parton level, absolute (left) and normalized (right), as a function of $m_{t\bar{t}}$. The bottom panel shows the ratio (theory - data).

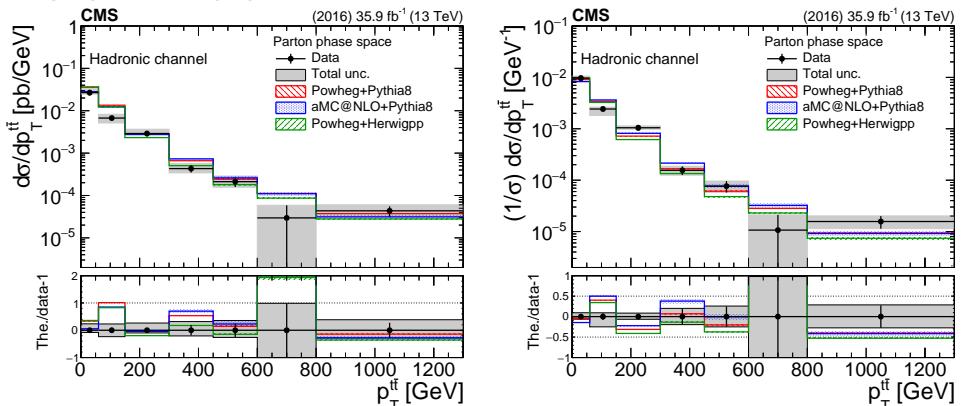


Figure 54: Differential cross section unfolded to parton level, absolute (left) and normalized (right), as a function of $p_T^{t\bar{t}}$. The bottom panel shows the ratio (theory - data).

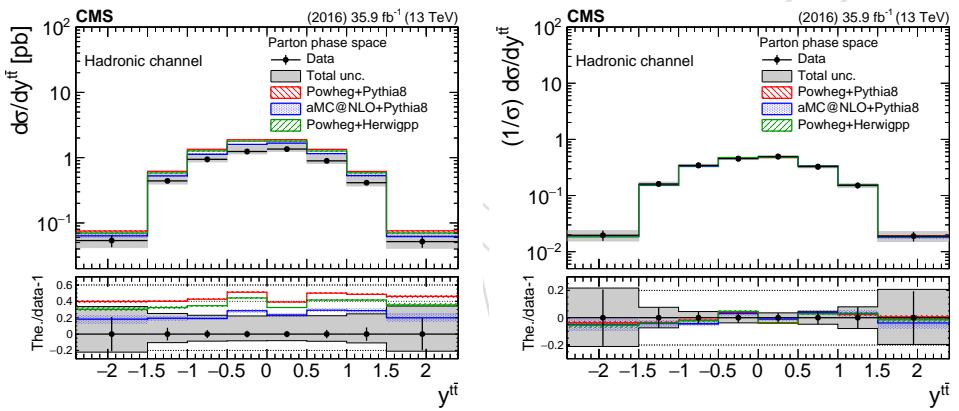


Figure 55: Differential cross section unfolded to parton level, absolute (left) and normalized (right), as a function of $y^{\bar{t}}$. The bottom panel shows the ratio (theory - data)/data.

9.2 Particle Level

The results of the unfolded measurement at particle level are shown in Figs. 60- 66. We observe that the uncertainties are similar to those of the parton level, while the comparison with the theory predictions follows the trends observed in the fiducial measurement. That is, there is an 20 – 40% lower inclusive cross section, while the shapes of the differential distributions are reasonably reproduced by all models. A hint of a deviation at very high values of $m^{t\bar{t}}$ is observed but the measurement is not very precise at this part of the phase space.

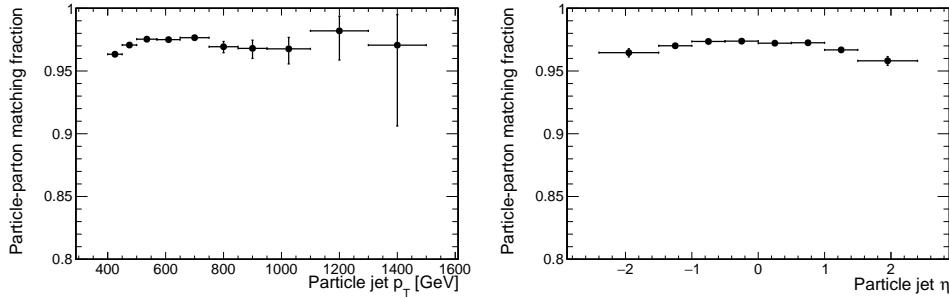


Figure 56: Simulated efficiency of the particle-level top candidates as a function of p_T and η .

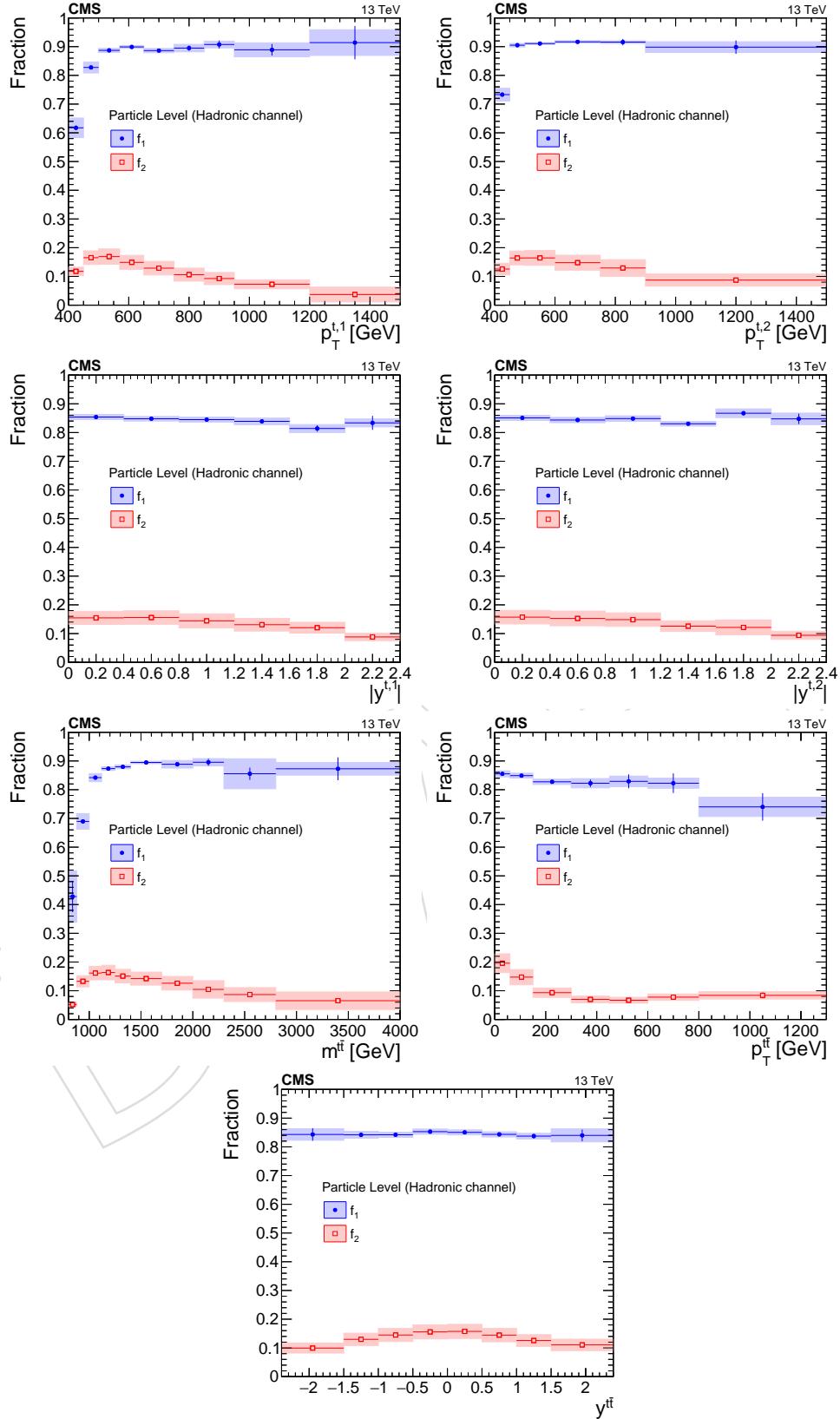


Figure 57: Simulated acceptance and efficiency for the particle-level selection as a function of the various observables.

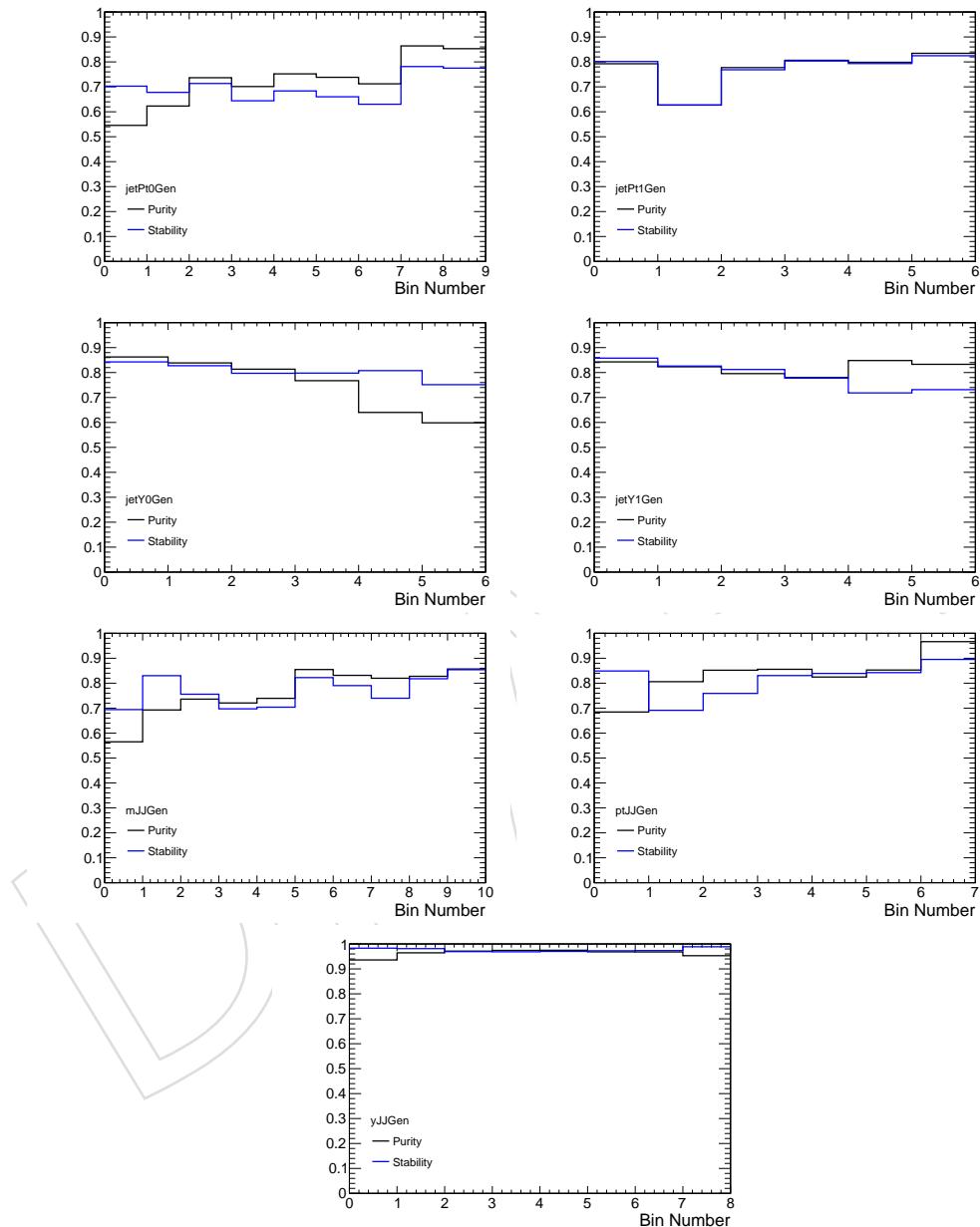


Figure 58: Simulated purity and stability of each bin at particle level.

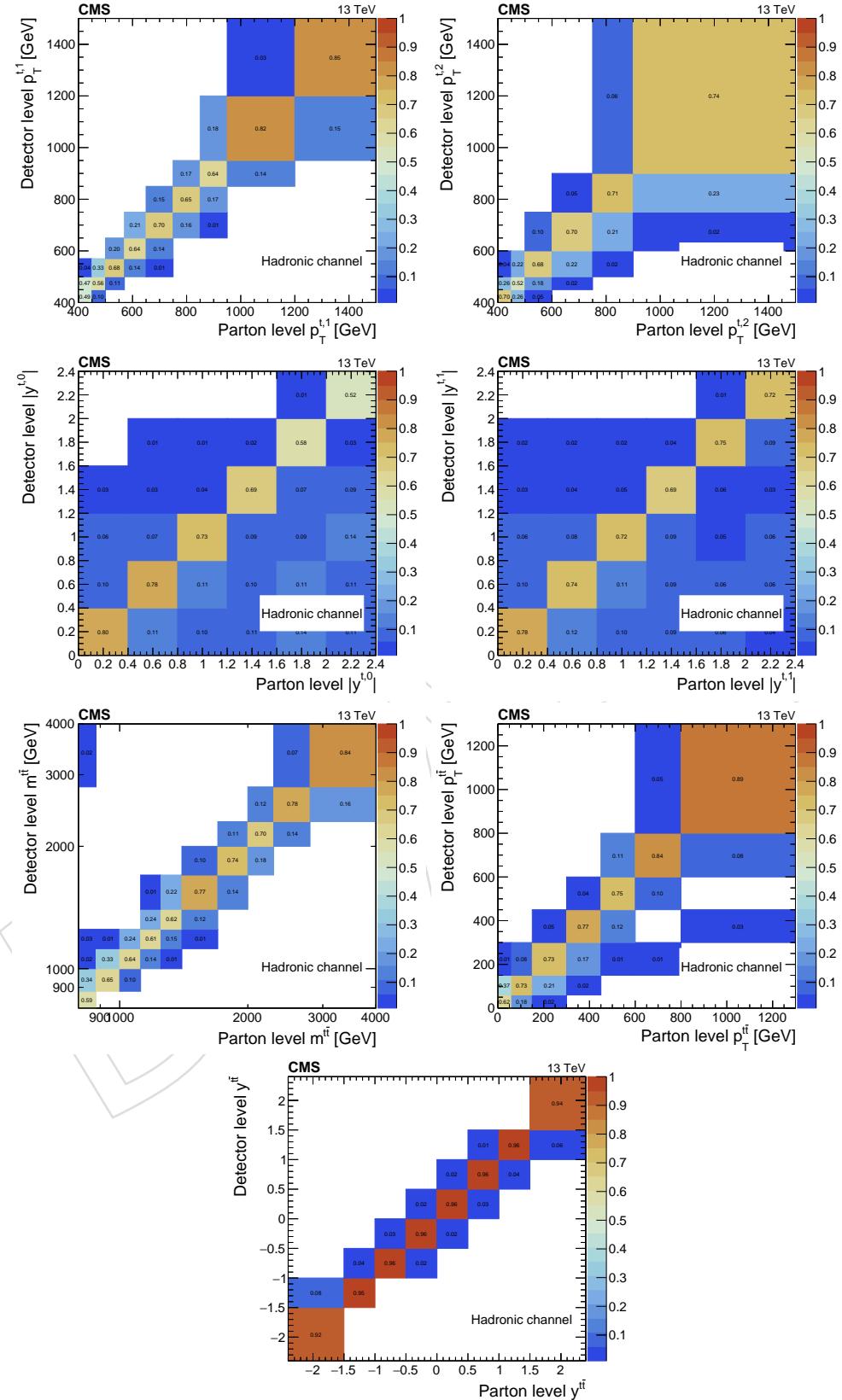


Figure 59: Simulated migration matrices at particle level. Each column is normalized to unity.

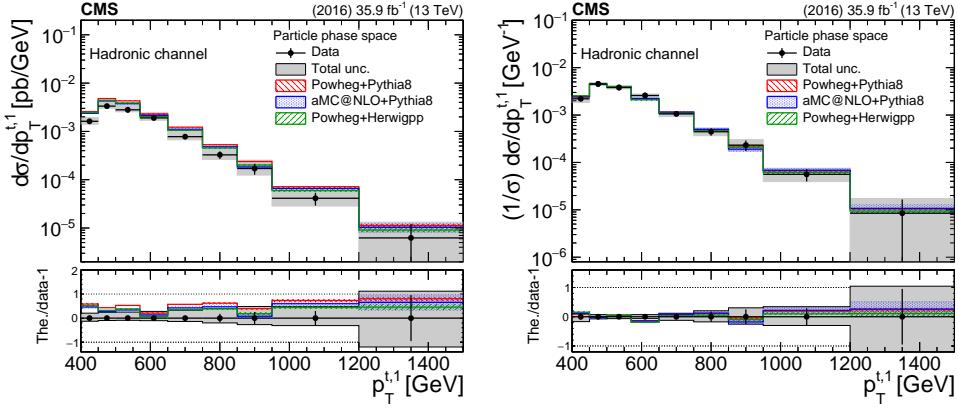


Figure 60: Differential cross section unfolded to particle level, absolute (left) and normalized (right), as a function of the leading top p_T . The bottom panel shows the ratio (theory - data)/data.

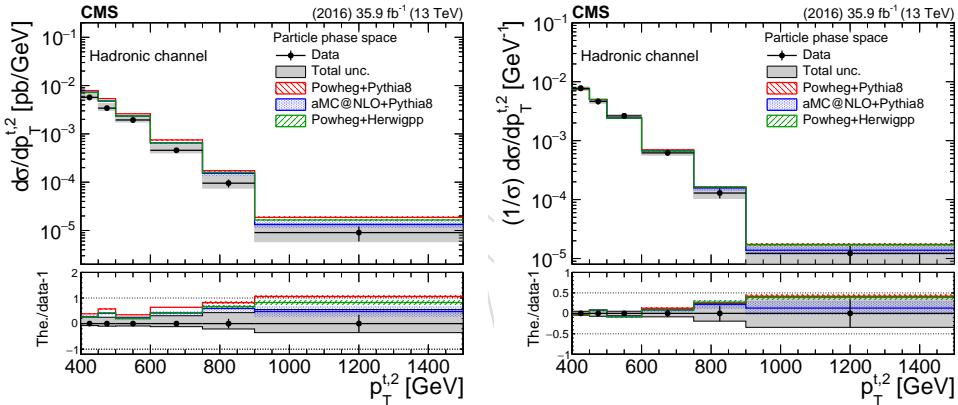


Figure 61: Differential cross section unfolded to particle level, absolute (left) and normalized (right), as a function of the second top p_T . The bottom panel shows the ratio (theory - data)/data.

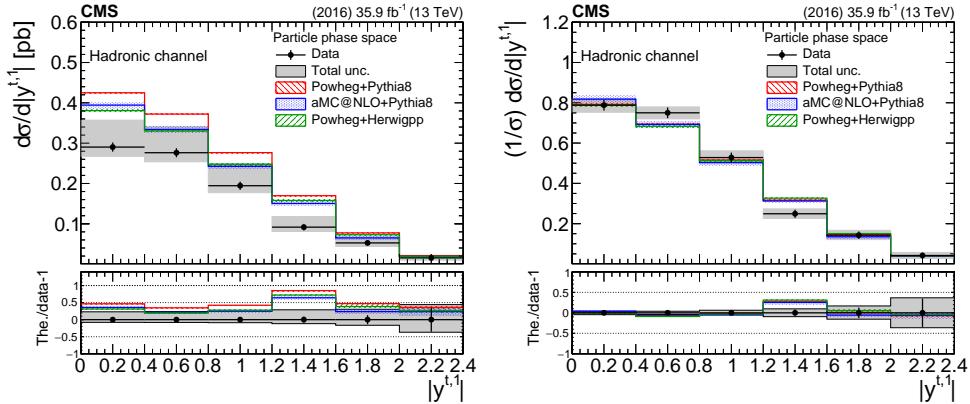


Figure 62: Differential cross section unfolded to particle level, absolute (left) and normalized (right), as a function of the leading top $|y|$. The bottom panel shows the ratio (theory - data)/data.

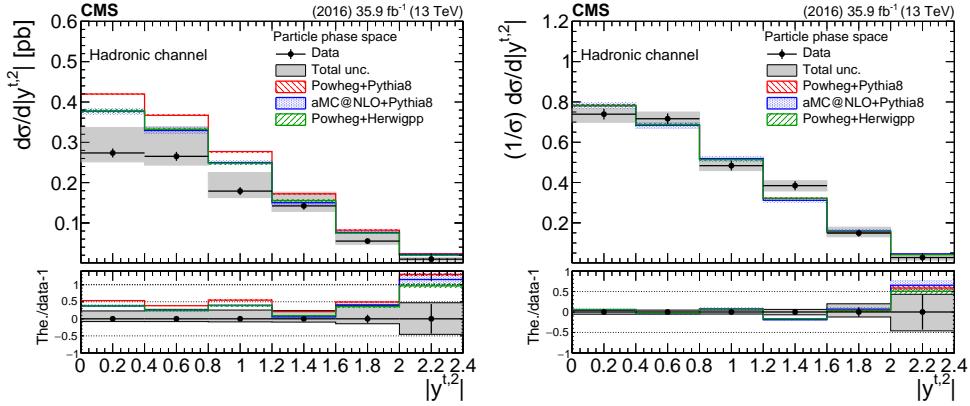


Figure 63: Differential cross section unfolded to particle level, absolute (left) and normalized (right), as a function of the leading top $|y|$. The bottom panel shows the ratio (theory - data)/data.

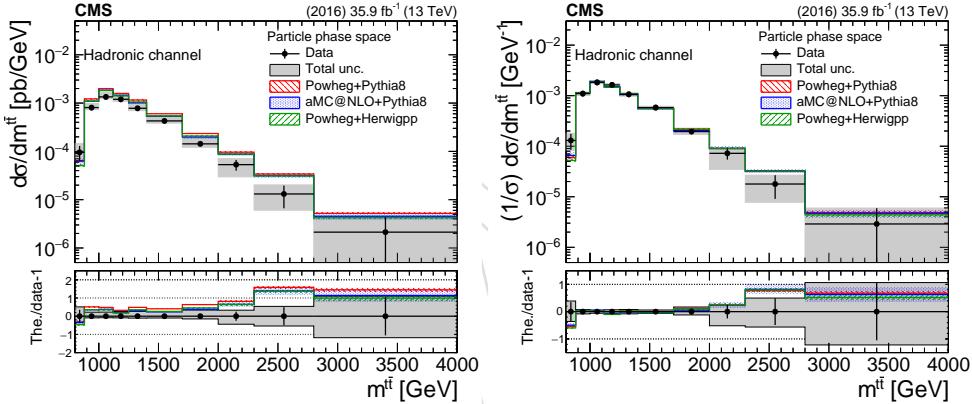


Figure 64: Differential cross section unfolded to particle level, absolute (left) and normalized (right), as a function of $m_{t\bar{t}}$. The bottom panel shows the ratio (theory - data)/data.

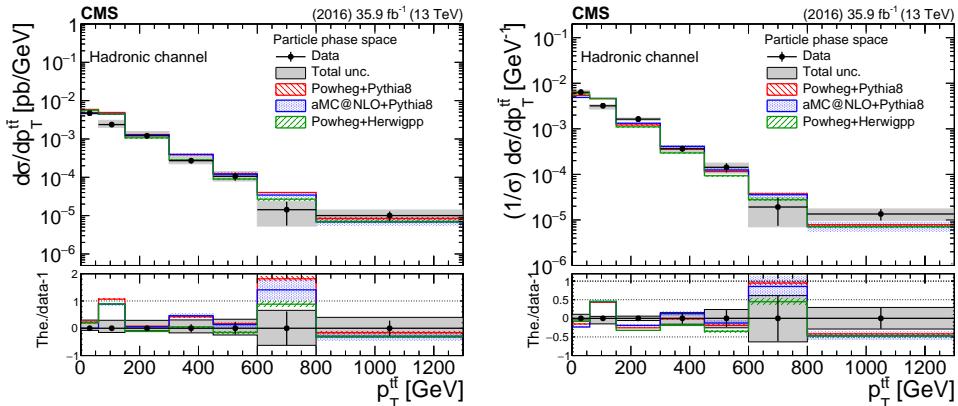


Figure 65: Differential cross section unfolded to particle level, absolute (left) and normalized (right), as a function of $p_T^{t\bar{t}}$. The bottom panel shows the ratio (theory - data)/data.

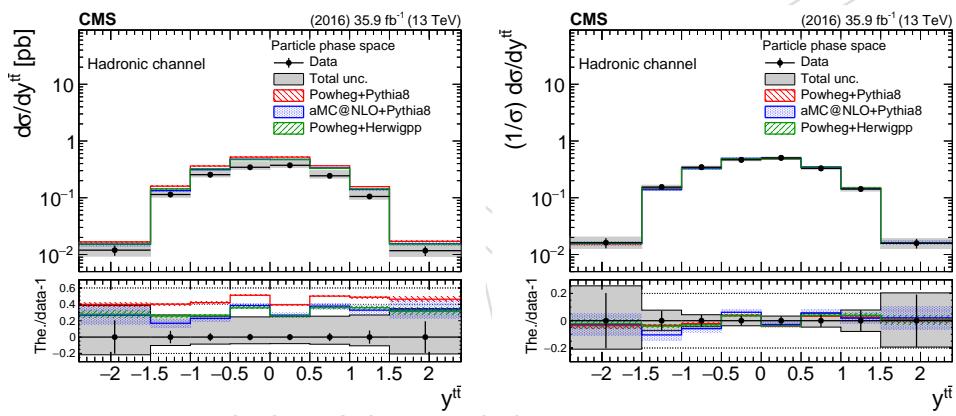


Figure 66: Differential cross section unfolded to particle level, absolute (left) and normalized (right), as a function of $y_{t\bar{t}}$. The bottom panel shows the ratio (theory - data)/data.

448 10 Summary

449 A measurement of the $t\bar{t}$ production cross section for high- p_T top quarks at 13 TeV proton-
450 proton collisions has been presented. The measurement is performed with events where both
451 top quarks decay hadronically, and where the hadronic decay products cannot be resolved but
452 are instead clustered in a single large- R jet with $p_T > 400$ GeV. The hadronic final state thus
453 contains two large- R jets. The cross section is reported differentially as a function of (inclusive)
454 top p_T and η , and as a function of the invariant mass, p_T , and rapidity of the $t\bar{t}$ system, un-
455 folded to the parton and particle levels, absolute and normalized. The results are compared
456 to theoretical predictions from the POWHEG matrix-element generator, interfaced with PYTHIA
457 8 or HERWIG ++ for the underlying event and parton shower, and from the MC@NLO matrix-
458 element generator, interfaced with PYTHIA 8. All the models overpredict significantly the ab-
459 solute cross section in the phase space of the measurement (up to 40%), while they are able
460 to describe consistently the differential shapes in all the variables. The most notable discrep-
461 ency can be seen in the invariant mass of the $t\bar{t}$ system, where the theoretical models predict
462 higher cross section at high mass values. However, in order to estimate the significance of the
463 discrepancy, more data are needed.



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595 $\sqrt{s} = 13$ TeV with the ATLAS Detector at the LHC", *Phys. Rev. Lett.* **117** (2016), no. 18,
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DRAFT

599 A Data vs simulation with default MC normalization

600 Below we show the data vs simulation comparisons for various observables where the MC pro-
 601 cesses are normalized according to the known cross sections, without using the postfit values
 602 for the $t\bar{t}$ and QCD yields.

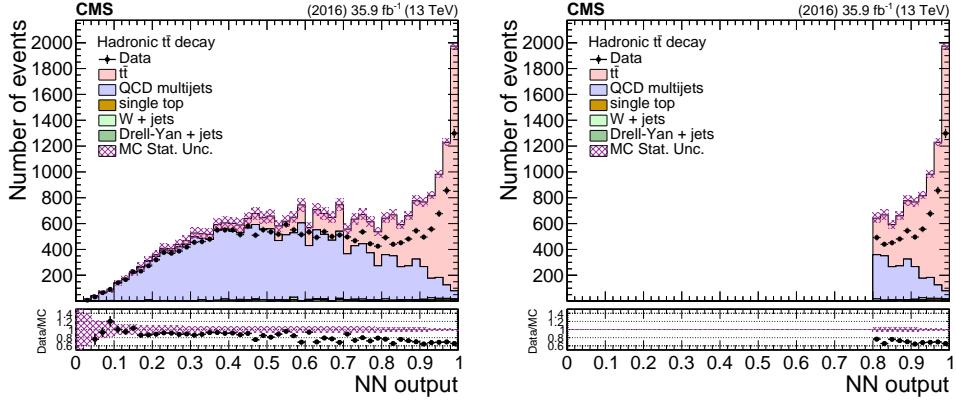


Figure 67: Data vs simulation before (left) and after (right) applying the $NN > 0.8$ cut for the NN output.

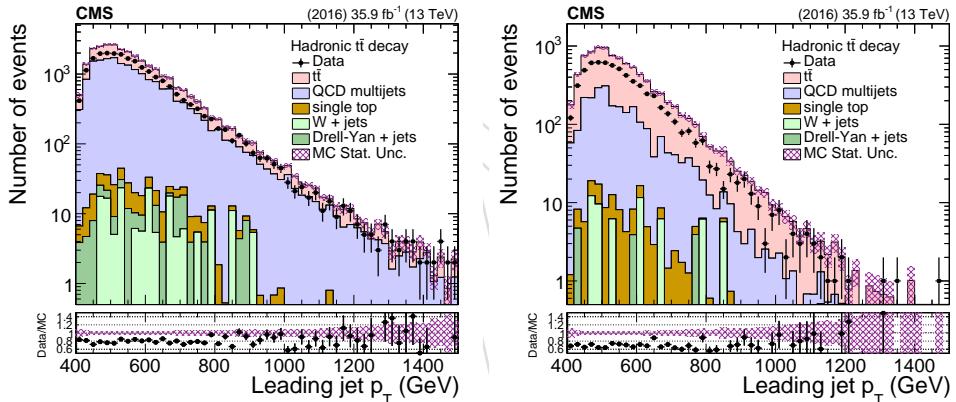


Figure 68: Data vs simulation before (left) and after (right) applying the $NN > 0.8$ cut for the p_T of the leading jet.

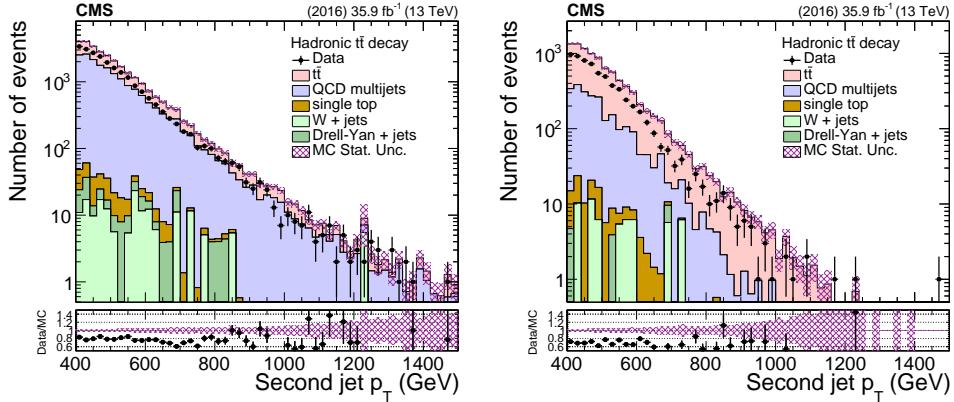


Figure 69: Data vs simulation before (left) and after (right) applying the $NN > 0.8$ cut for the p_T of the second jet.

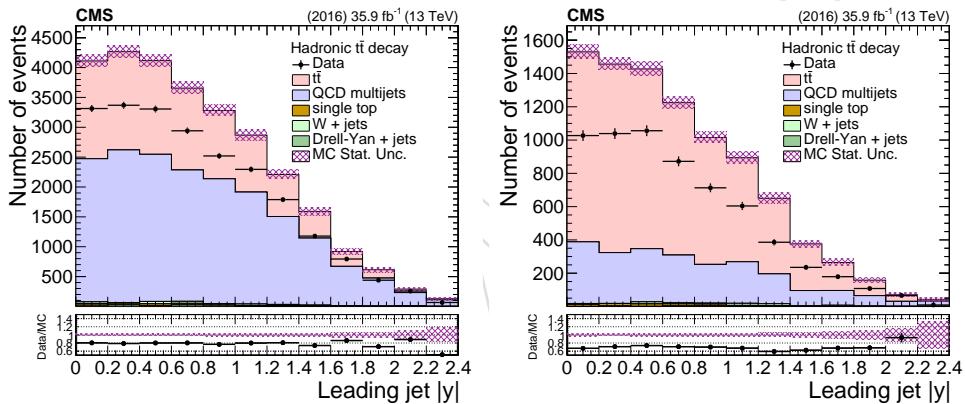


Figure 70: Data vs simulation before (left) and after (right) applying the $NN > 0.8$ cut for the $|y|$ of the leading jet.

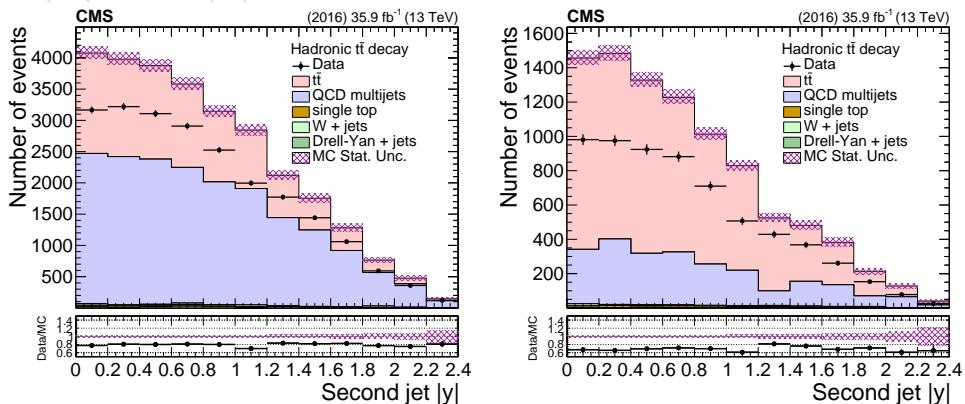


Figure 71: Data vs simulation before (left) and after (right) applying the $NN > 0.8$ cut for the $|y|$ of the second jet.

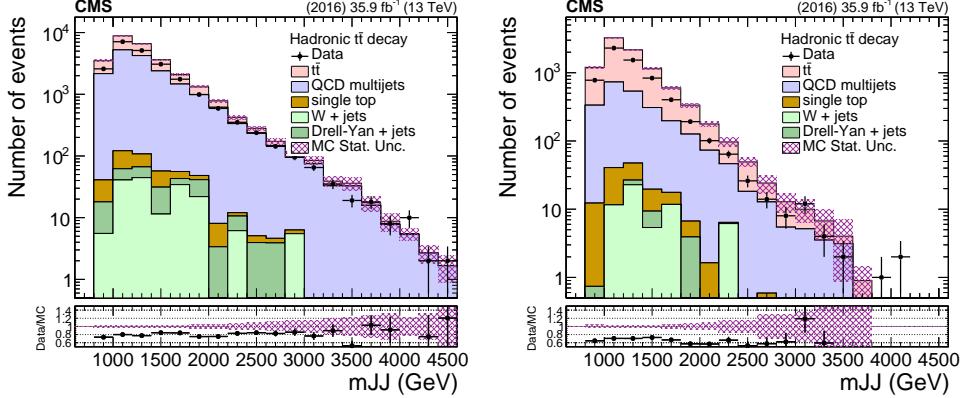


Figure 72: Data vs simulation before (left) and after (right) applying the $NN > 0.8$ cut for the mass of the $t\bar{t}$ system.

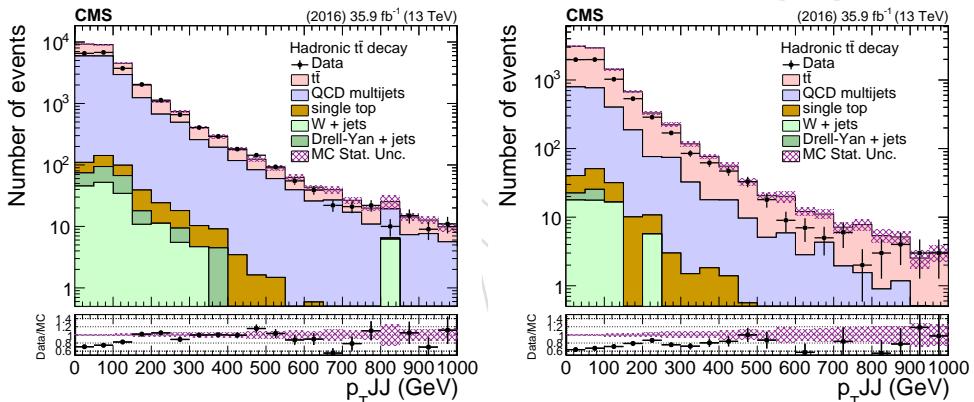


Figure 73: Data vs simulation before (left) and after (right) applying the $NN > 0.8$ cut for the p_T of the $t\bar{t}$ system.

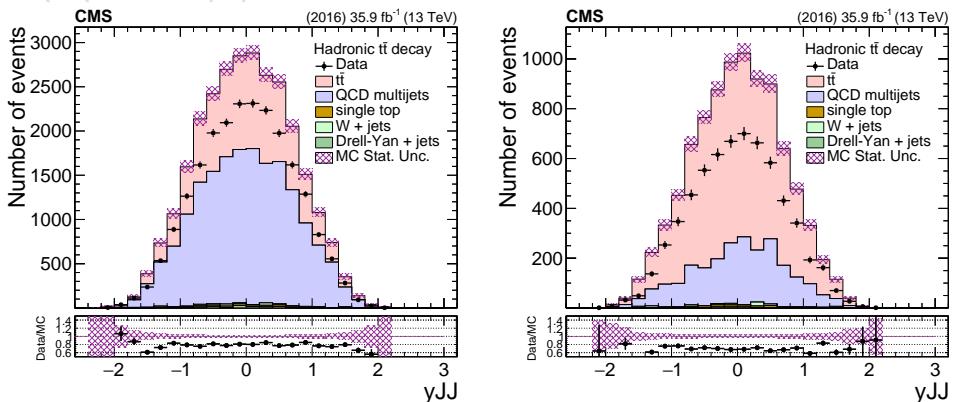


Figure 74: Data vs simulation before (left) and after (right) applying the $NN > 0.8$ cut for the rapidity of the $t\bar{t}$ system.

603 B NN Input Variables

604 In this section we provide additional comparisons between data and simulation for the six
 605 variables used as inputs for the NN training, in three different categories: 0, 1, or 2 top jet
 606 candidates with a b tagged subjet, prior any cut on the NN output.

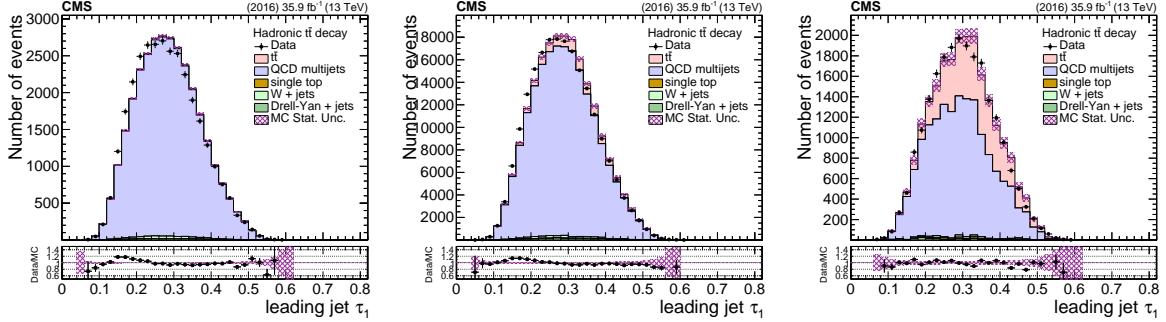


Figure 75: Data vs simulation for the τ_1 variable of the leading jet after the selection of 0 btagged subjet (left), 1 (middle) and 2 (right).

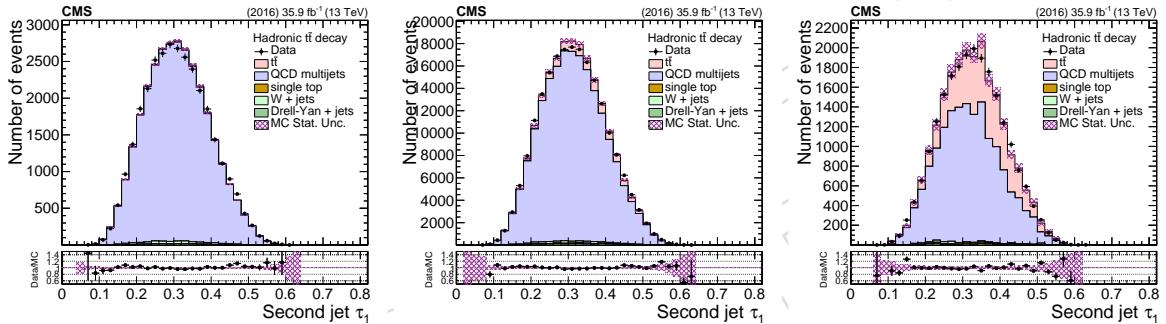


Figure 76: Data vs simulation for the τ_1 variable of the second jet after the selection of 0 btagged subjet (left), 1 (middle) and 2 (right).

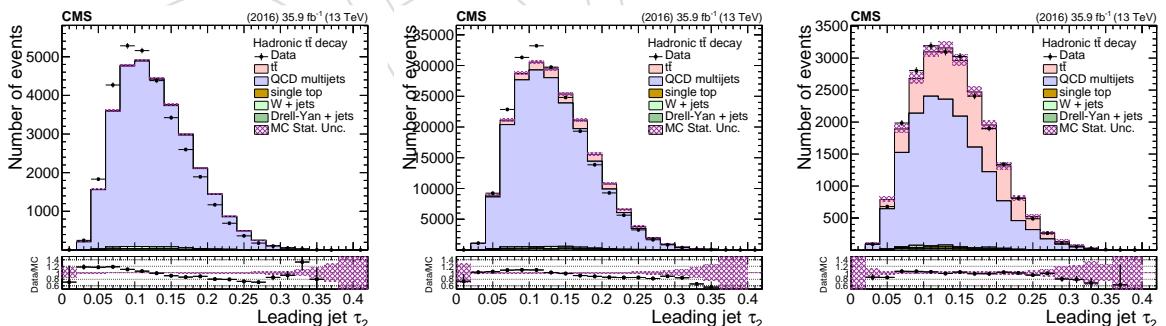


Figure 77: Data vs simulation for the τ_2 variable of the leading jet after the selection of 0 btagged subjet (left), 1 (middle) and 2 (right).

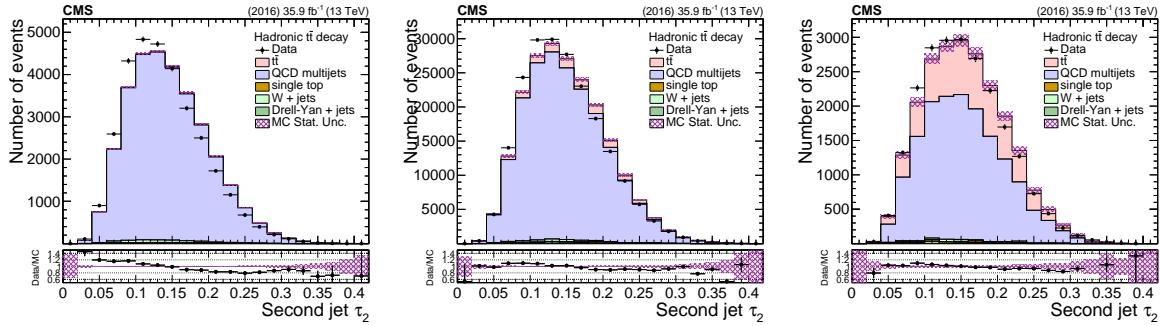


Figure 78: Data vs simulation for the τ_2 variable of the second jet after the selection of 0 btagged subjet (left), 1 (middle) and 2 (right).

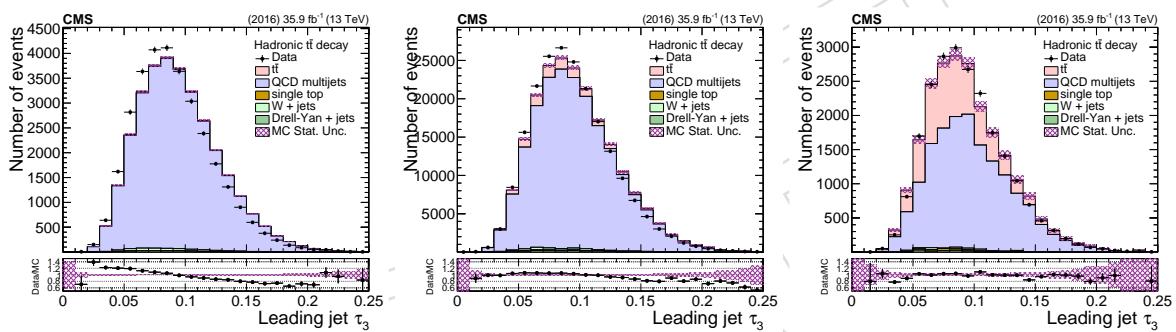


Figure 79: Data vs simulation for the τ_3 variable of the leading jet after the selection of 0 btagged subjet (left), 1 (middle) and 2 (right).

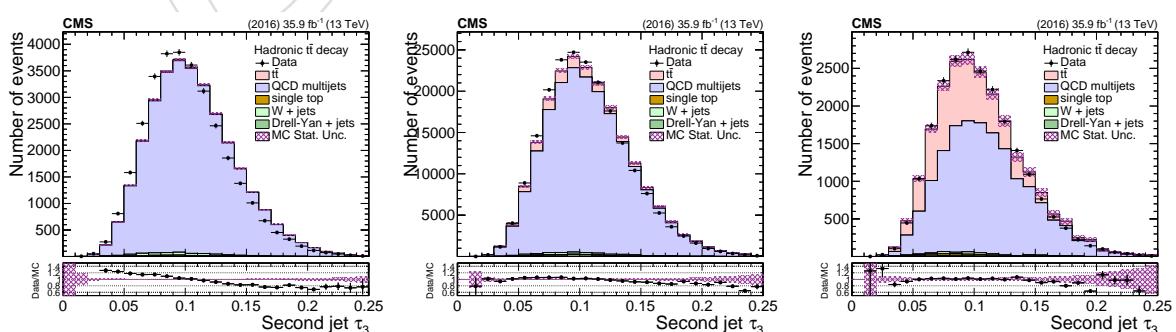


Figure 80: Data vs simulation for the τ_3 variable of the second jet after the selection of 0 btagged subjet (left), 1 (middle) and 2 (right).

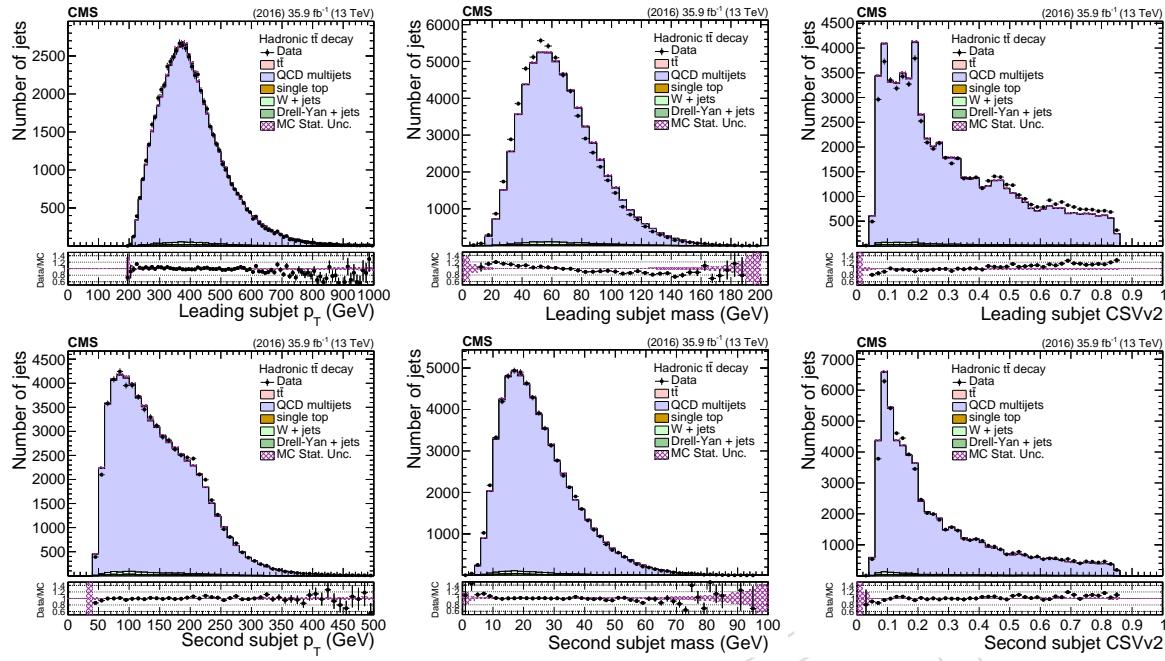


Figure 81: Data vs simulation for the p_T , mass, and CSVv2 variables for the two subjets of the top candidates after the baseline selection and the requirement of 0 b tagged subjets.

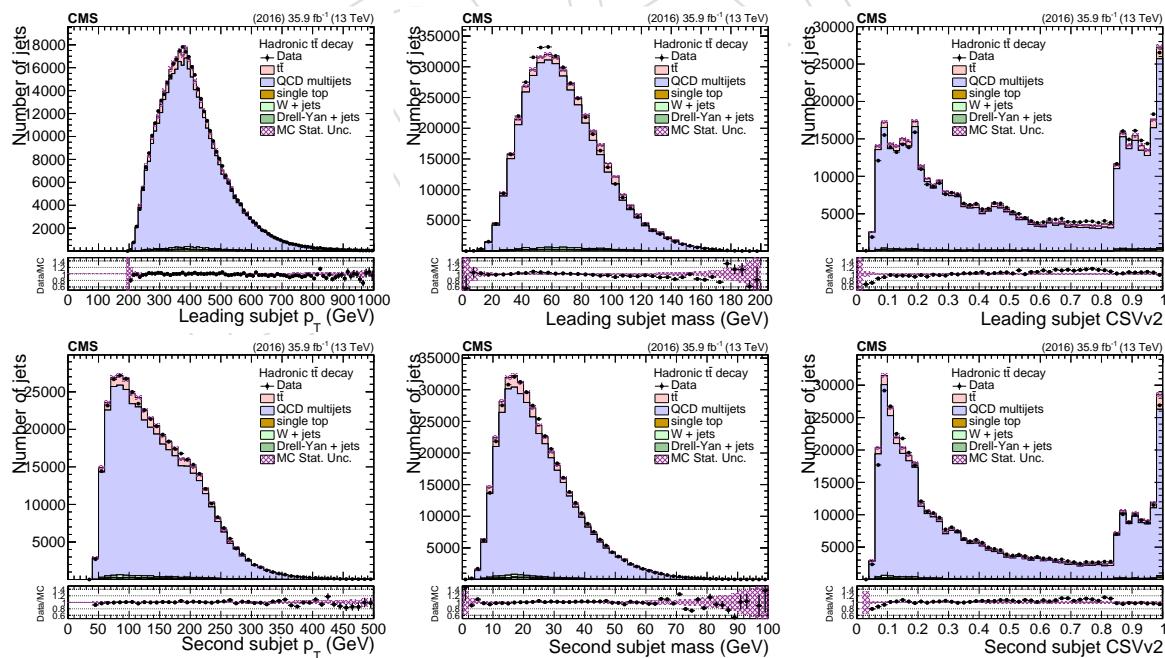


Figure 82: Data vs simulation for the p_T , mass, and CSVv2 variables for the two subjets of the top candidates after the baseline selection and the requirement of 1 b tagged subjets.

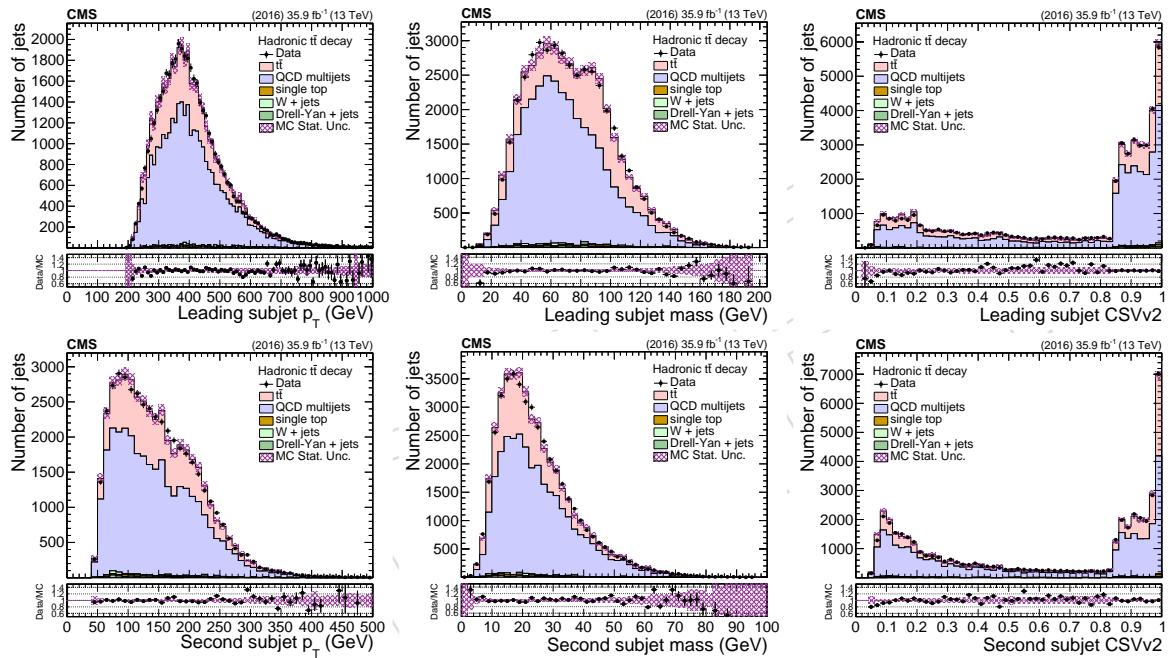


Figure 83: Data vs simulation for the p_T , mass, and CSVv2 variables for the two subjets of the top candidates after the baseline selection and the requirement of 2 b tagged subjets.

607 C Control Distributions

608 In this section we provide additional comparisons between data and simulation. In what fol-
 609 lows, we show the various observables in the control and signal regions.

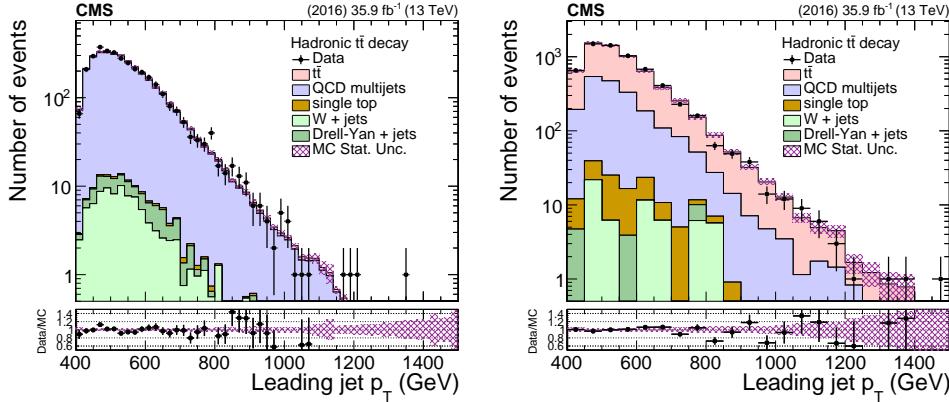


Figure 84: Data vs simulation in the control (left) and signal (right) regions for the p_T of the two leading jets.

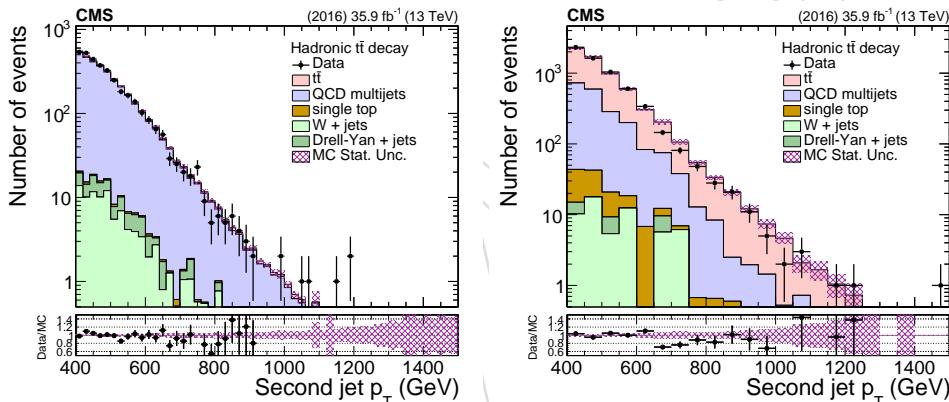


Figure 85: Data vs simulation in the control (left) and signal (right) regions for the p_T of the two leading jets.

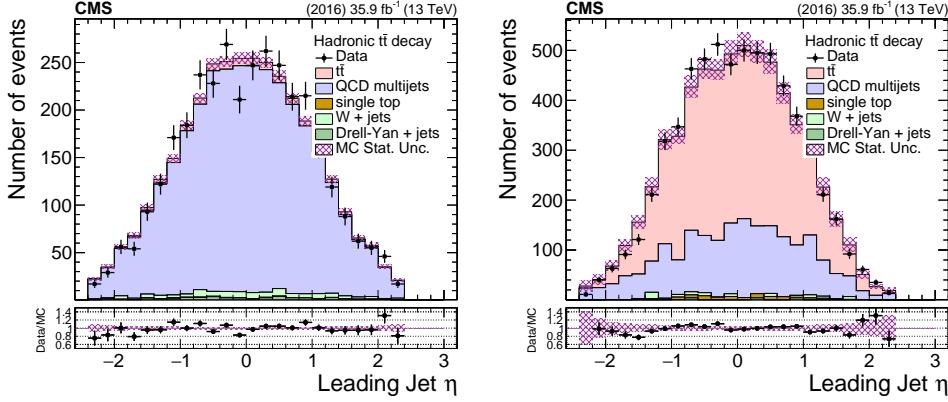


Figure 86: Data vs simulation in the control (left) and signal (right) regions for the η of the two leading jets.

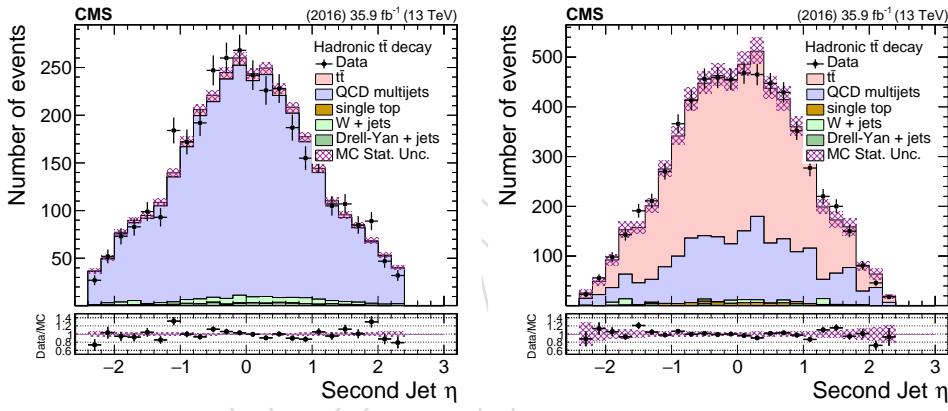


Figure 87: Data vs simulation in the control (left) and signal (right) regions for the η of the two leading jets.

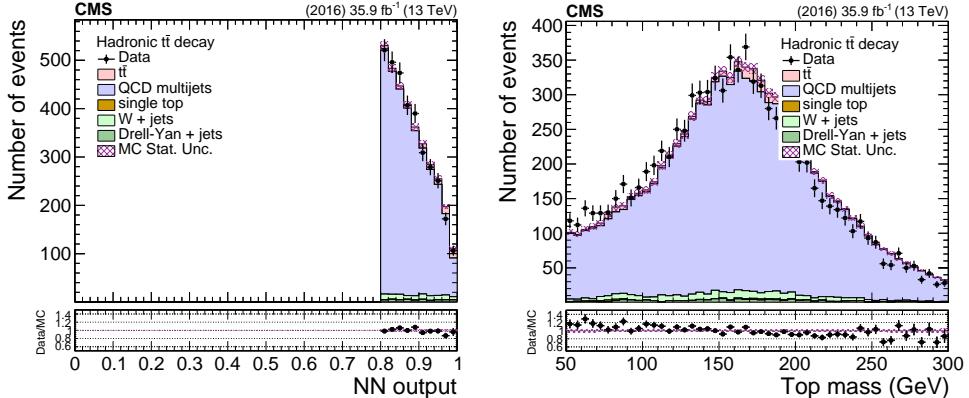


Figure 88: Data vs simulation in the control region for the NN output (left) and the top mass estimator (right).

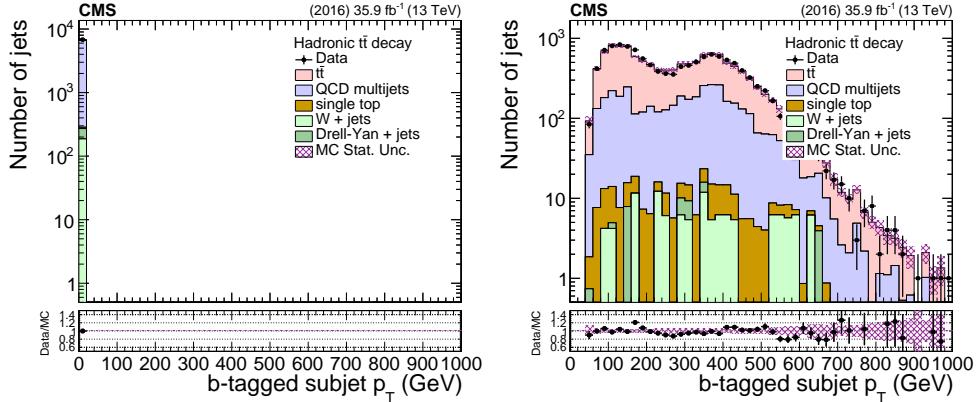


Figure 89: Data vs simulation in the control (left) and signal (right) regions for the p_T of the b-tagged subjet of the two leading jets.

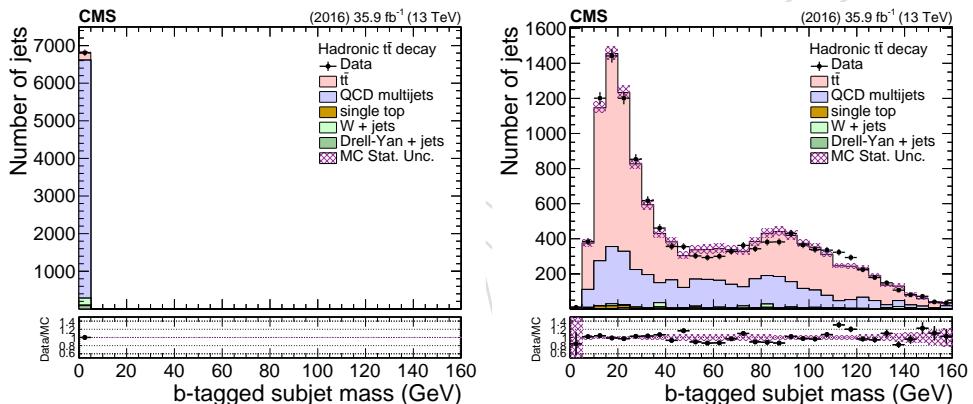


Figure 90: Data vs simulation in the control (left) and signal (right) regions for the mass of the b-tagged subjet of the two leading jets.

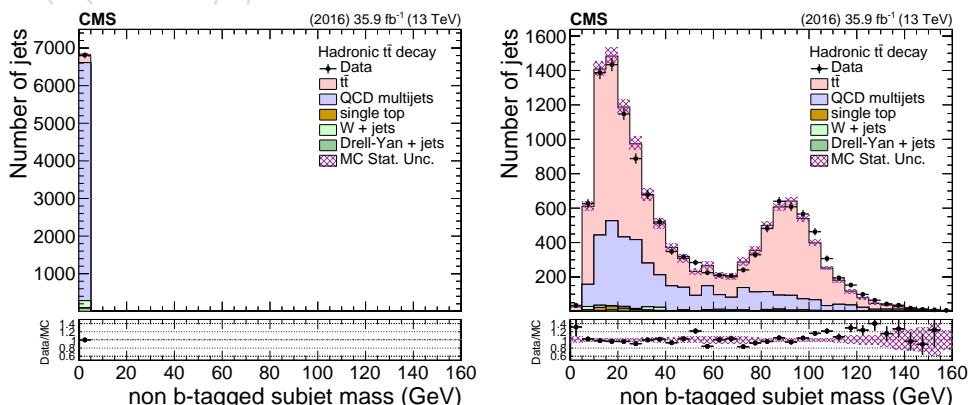


Figure 91: Data vs simulation in the control (left) and signal (right) regions for the mass of the non b-tagged subjet of the two leading jets.

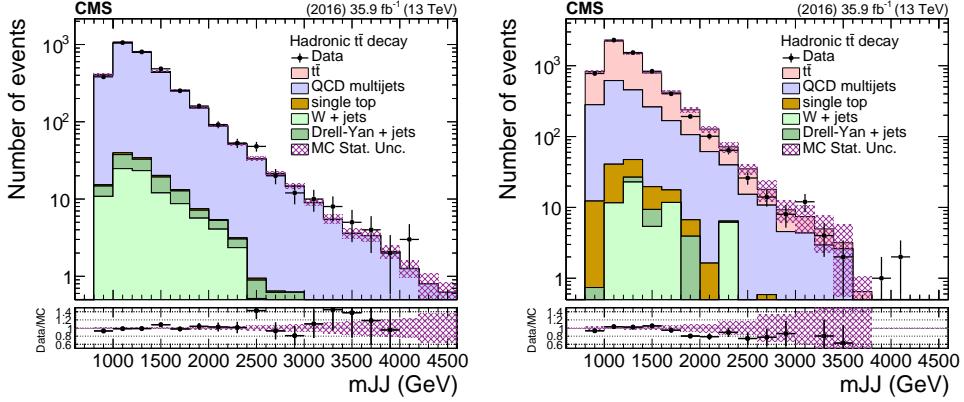


Figure 92: Data vs simulation in the control (left) and signal (right) regions dijet invariant mass.

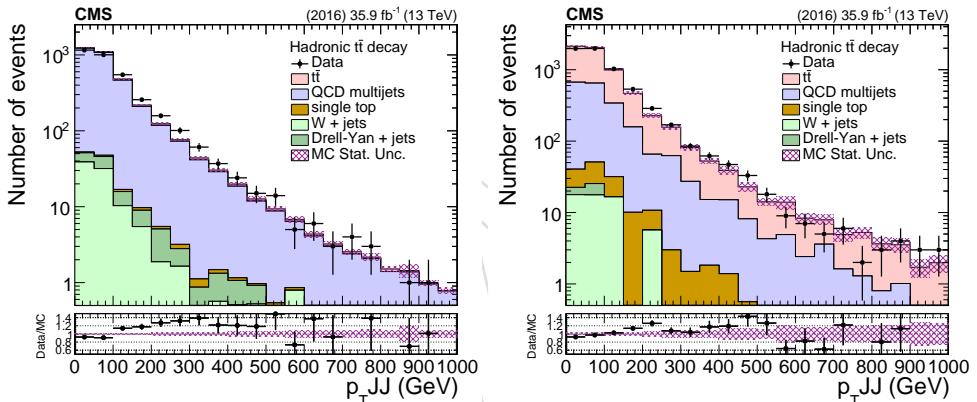


Figure 93: Data vs simulation in the control (left) and signal (right) regions dijet p_T .

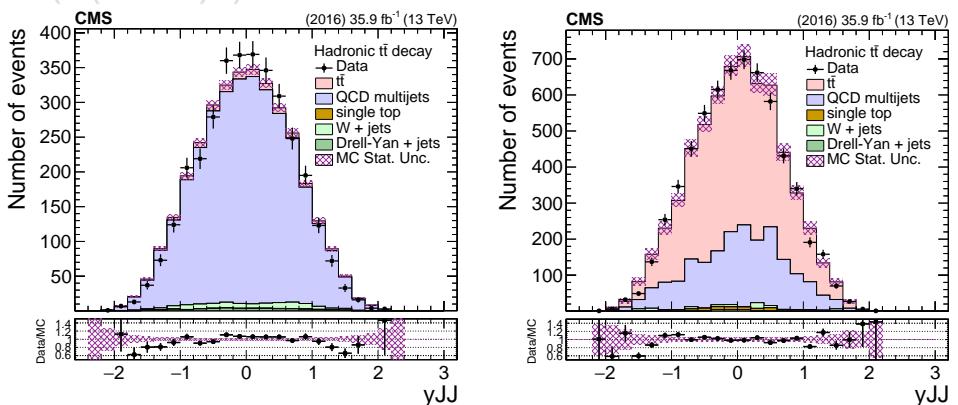


Figure 94: Data vs simulation in the control (left) and signal (right) regions dijet rapidity.

610 D Background Sensitivity to Pileup

611 The QCD background shape is taken from the corresponding control region in data, as de-
 612 scribed in Section 5. Since the data are collected with a prescaled trigger path, the pileup profile
 613 is different from the one of the signal events (Fig. 1). In order to demonstrate the robustness
 614 of the QCD prediction between the signal and control regions, we have performed the follow-
 615 ing test: the data from the control region are split in two subsets according to the number of
 616 reconstructed vertices (< 15 and ≥ 15) and we compare in Fig. 95 the distributions of the ob-
 617 servables used in this analysis. A systematic difference is observed in the softdrop mass of the
 618 jets, which is expected to be the most sensitive to pileup. This difference is naturally accounted
 619 for in the extraction of the QCD normalization (Eq. 2) with the unconstrained nuisance param-
 620 eter k_{slope} . In contrast, the shape of the jet and dijet kinematic observables are fully compatible
 621 within the statistical uncertainty. Therefore, taking also into account that the difference of the
 622 pileup profile of the two trigger paths is not as extreme as the test conducted here, we conclude
 623 that no significant bias is introduced by using the QCD shapes from the control region.

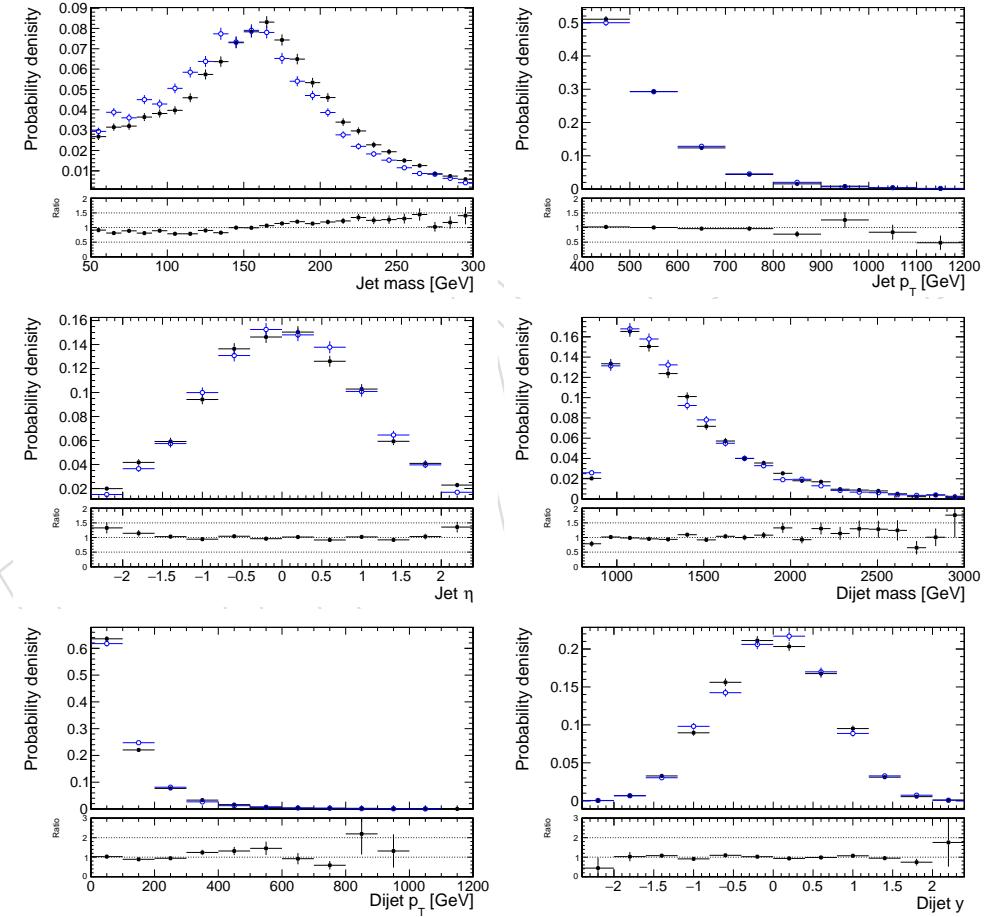


Figure 95: Distributions of jet and dijet observables from low pileup events (black, $\text{nvtx} < 15$) and high pileup events (blue, $\text{nvtx} \geq 15$). The bottom panel shows the ratio of the two.

624 **E Unfolding Tests**

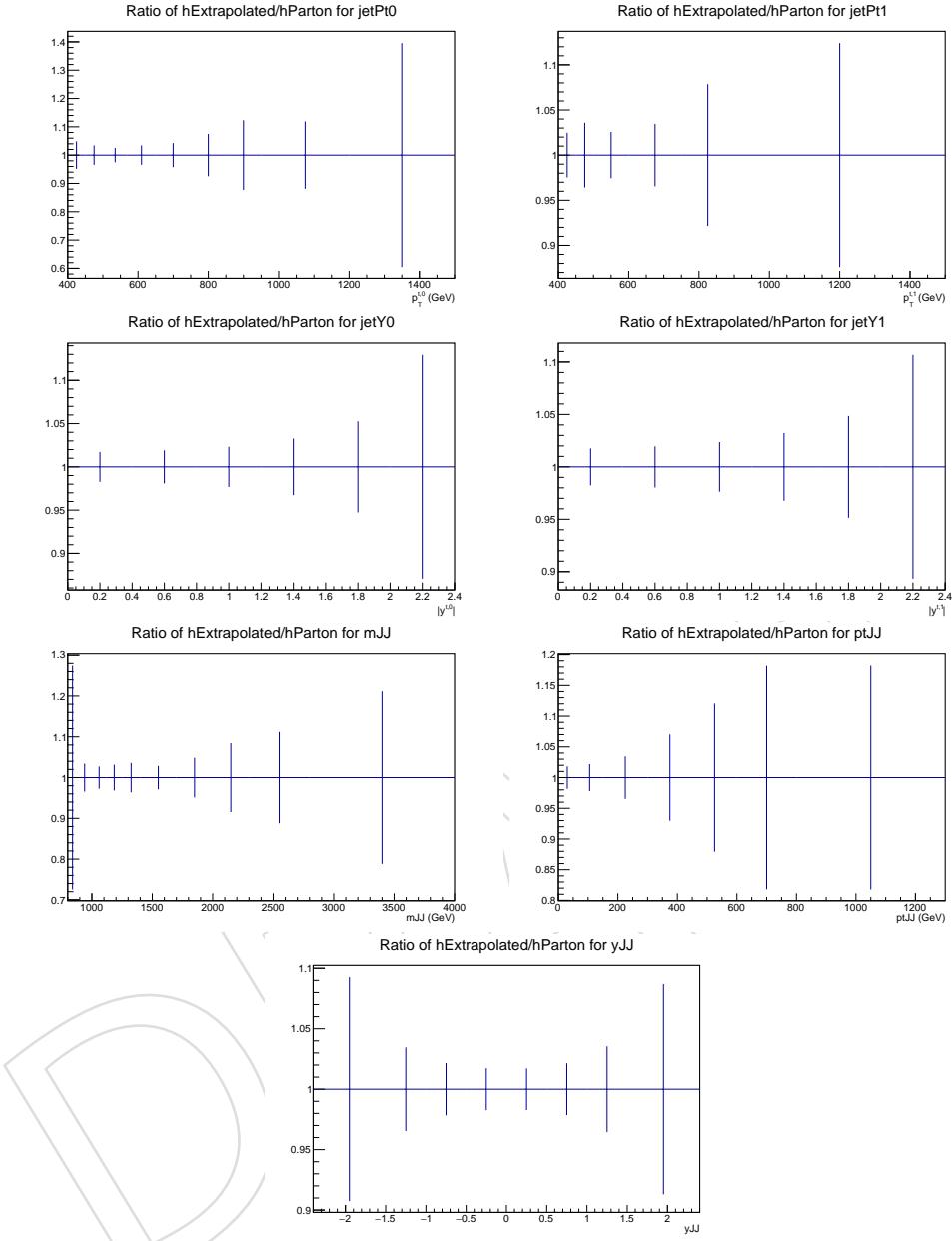


Figure 96: Parton unfolding closure test in simulation for all the reported observables. Ratio of the unfolded over the parton spectra.

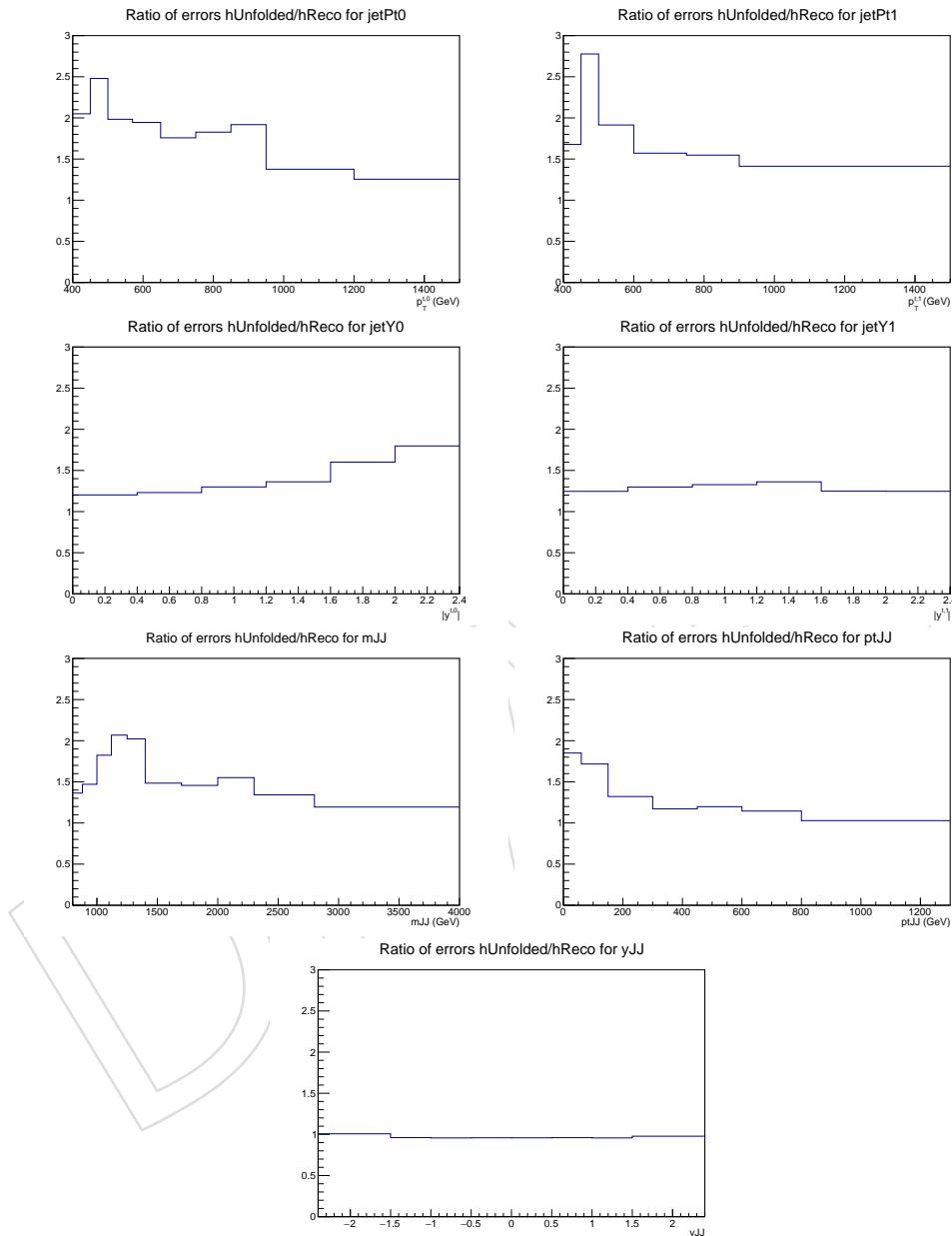


Figure 97: Ratio of the unfolded of the measured relative statistical uncertainties in the simulation (parton level).

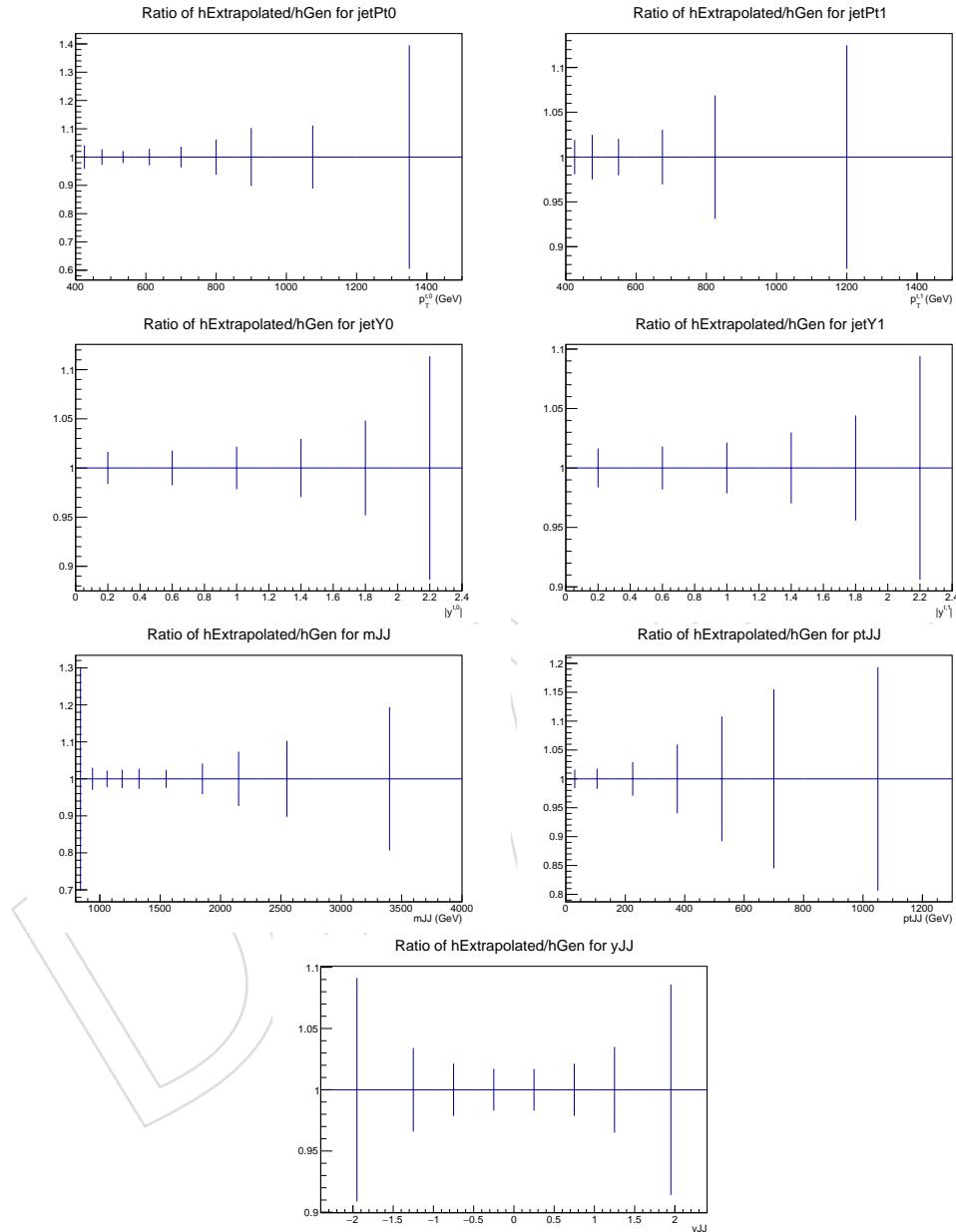


Figure 98: Particle unfolding closure test in simulation for all the reported observables. Ratio of the unfolded over the particle spectra.

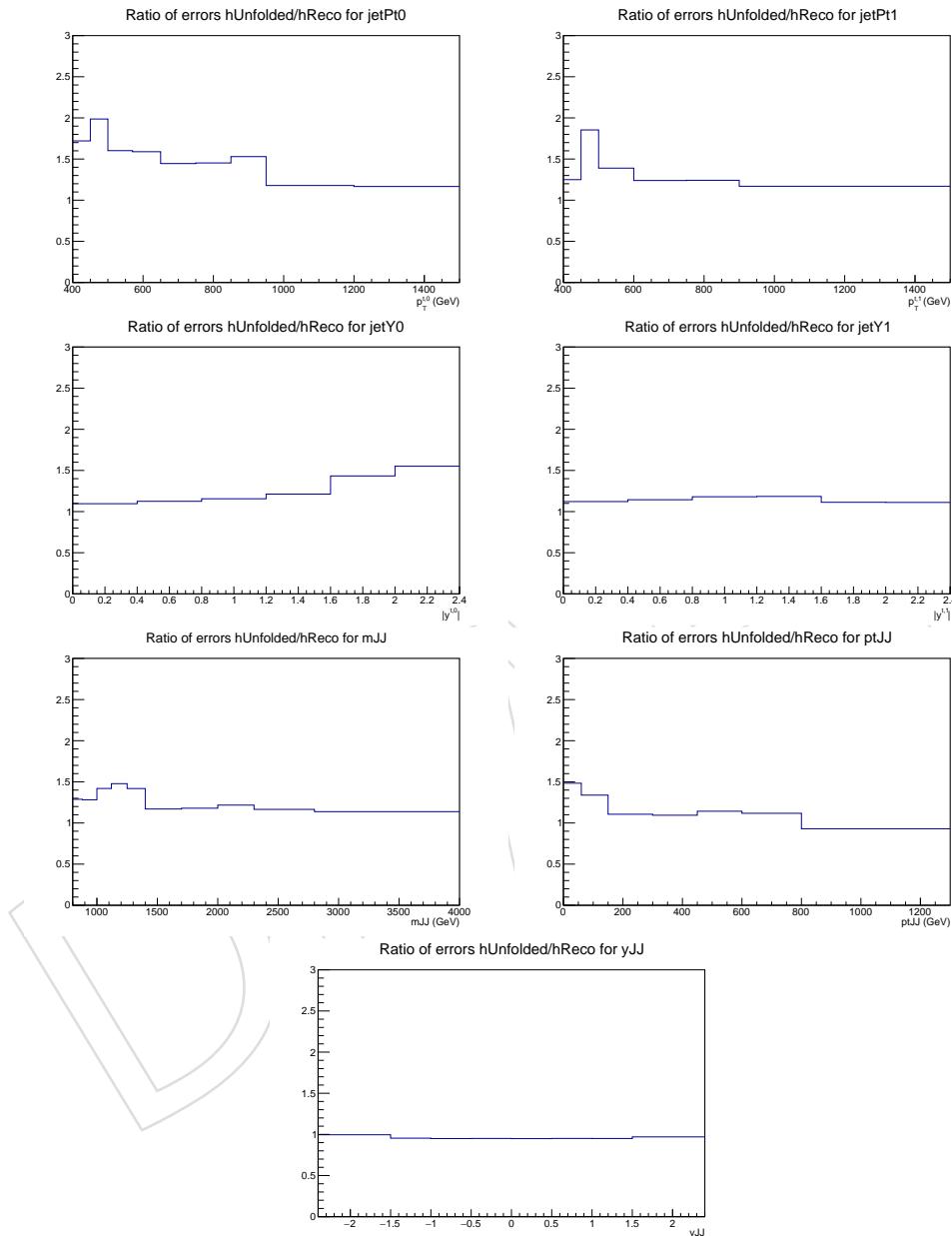


Figure 99: Ratio of the unfolded of the measured relative statistical uncertainties in the simulation (particle level).

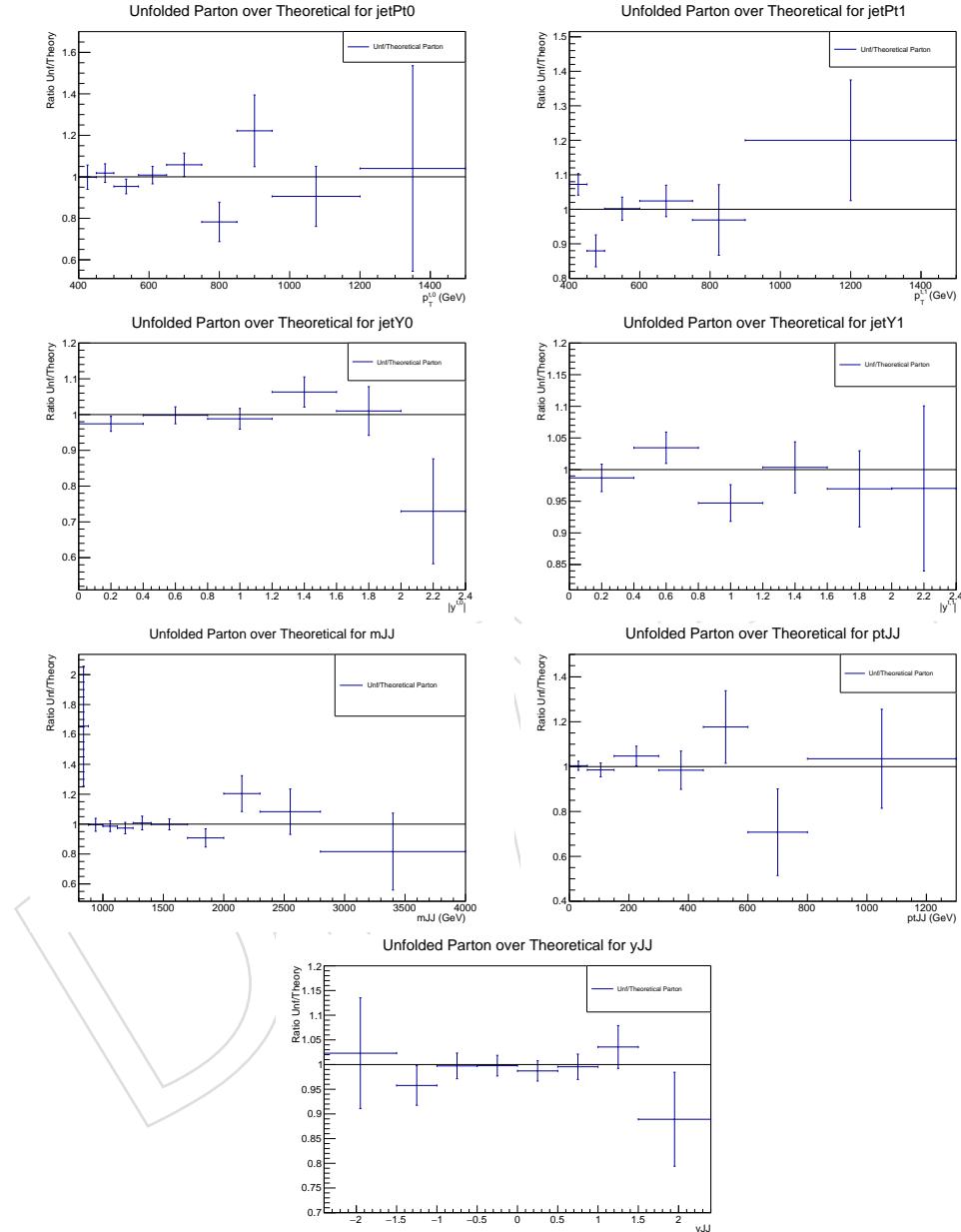


Figure 100: Stability of the unfolding at parton level in the simulation. The response matrix is derived from the first half of the sample and applied to the other half.

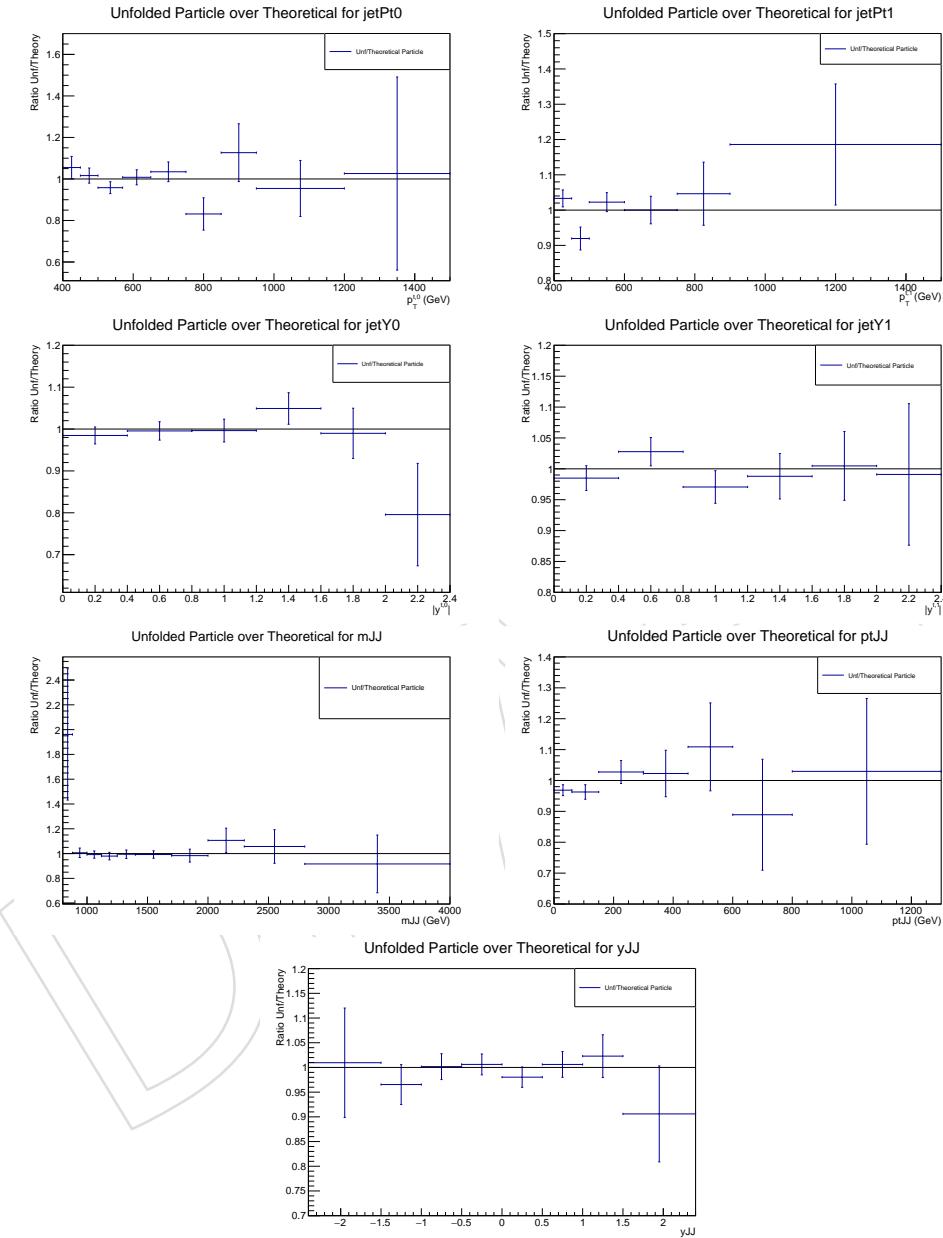


Figure 101: Stability of the unfolding at particle level in the simulation. The response matrix is derived from the first half of the sample and applied to the other half.

625 F Simulated b tagging efficiencies

626 In this section we show the b tagging efficiency of subjets for each parton in Fig. 102 and the
 627 purity of the b tagged reconstructed subjets in Fig. 103.

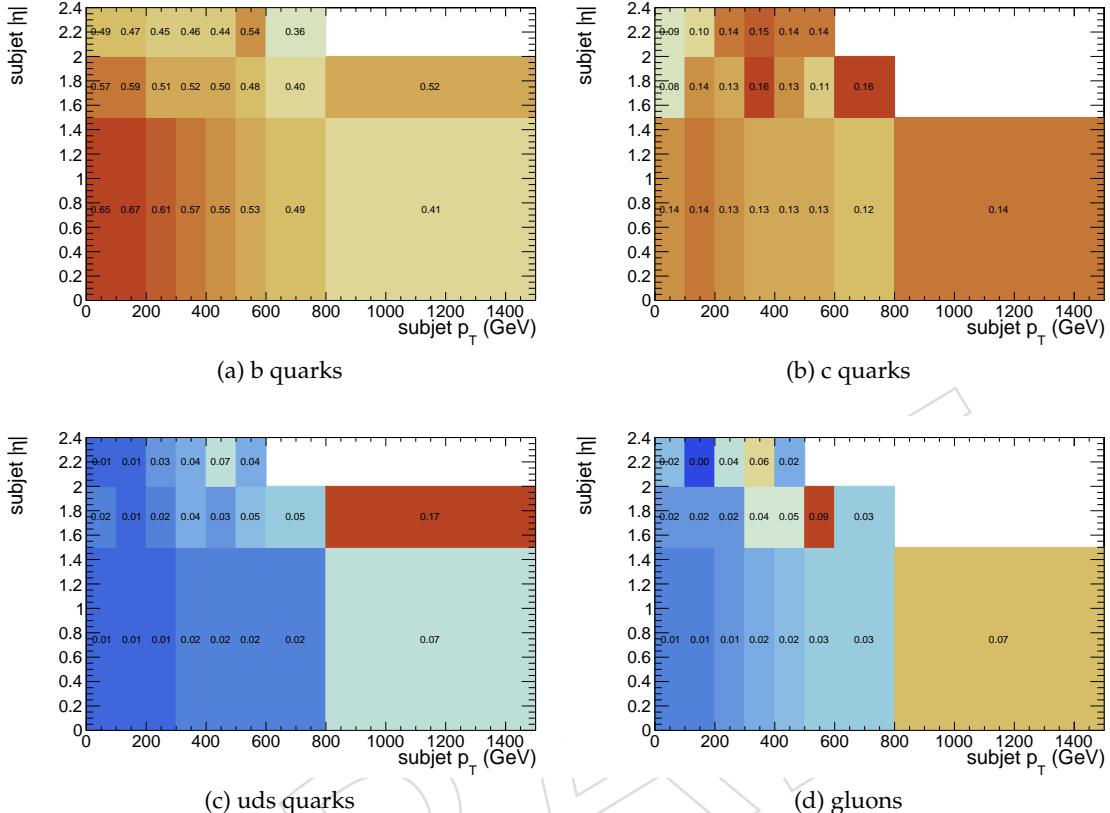


Figure 102: Simulated b tagging efficiency of subjets for different parton types.

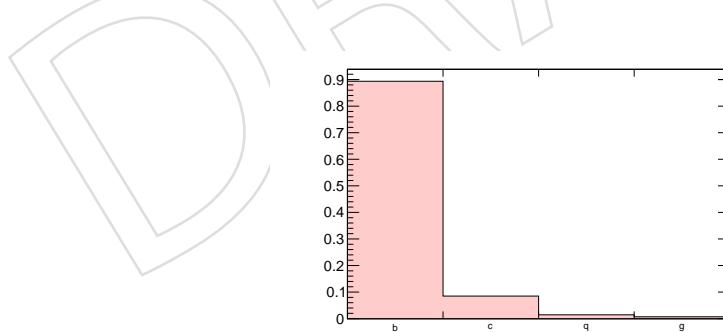


Figure 103: Distribution of the parton flavor for each b tagged subjet.

628 G Correlation Matrices

629 In this section we present the **correlation matrices** between the bins of the unfolded distribu-
 630 tions.

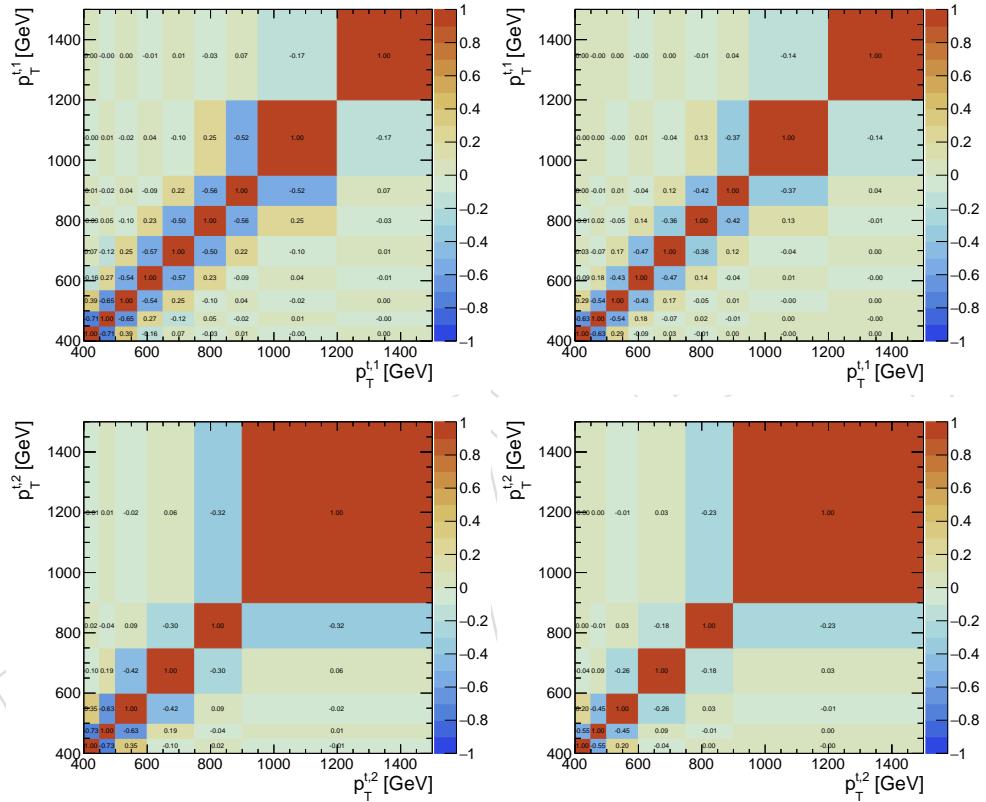


Figure 104: Correlation matrices for the unfolded top p_T distributions at parton (left) and particle (right) level.

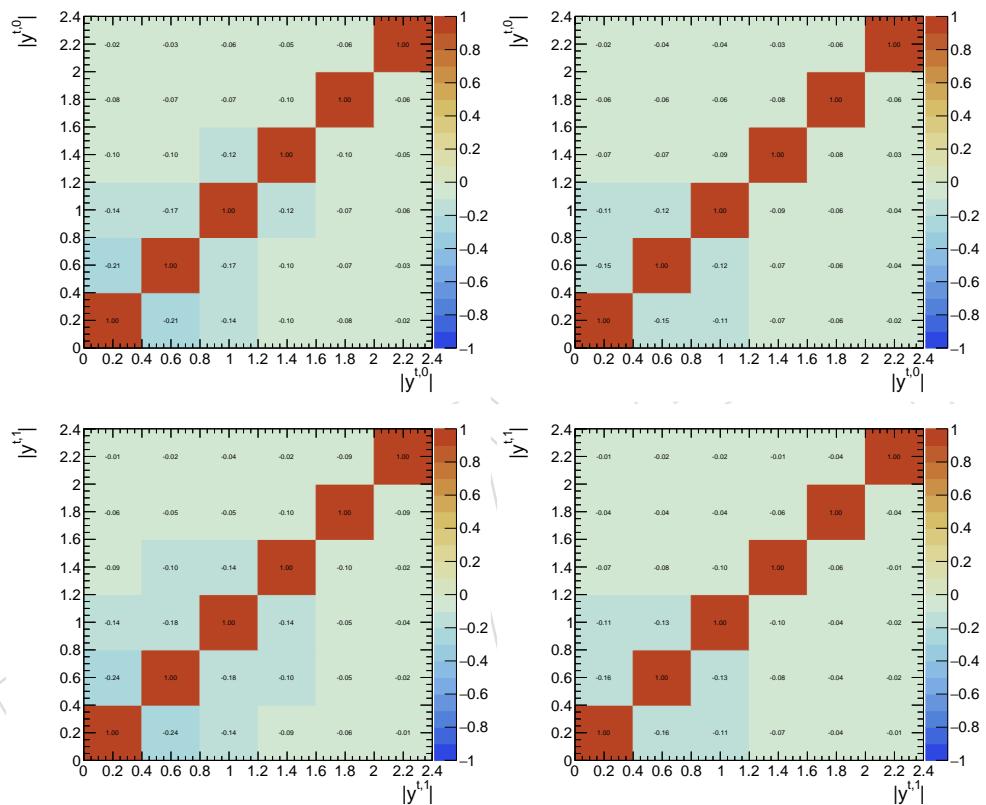


Figure 105: Correlation matrices for the unfolded top $|y|$ distributions at parton (left) and particle (right) level.

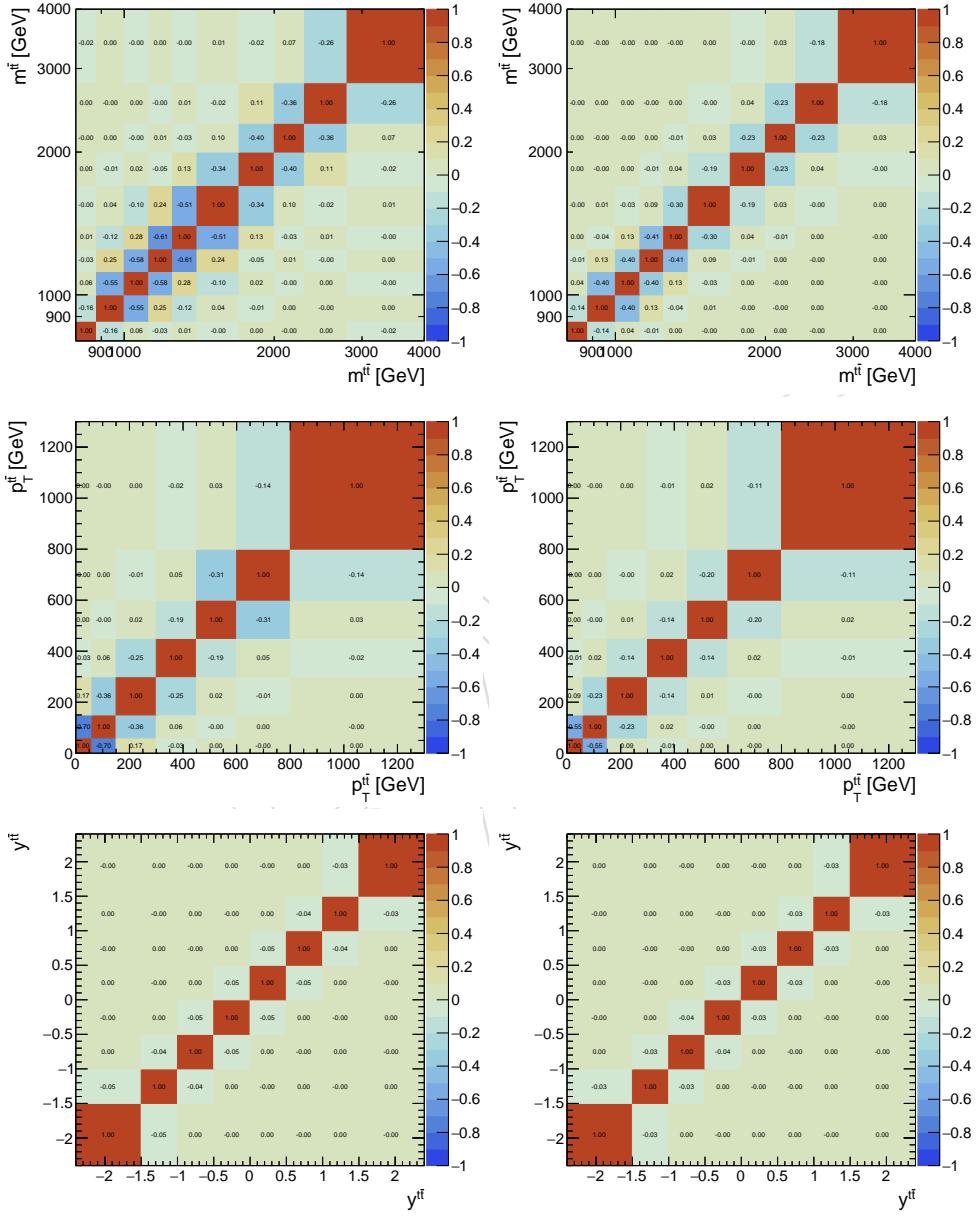


Figure 106: Correlation matrices for the unfolded $t\bar{t}$ distributions at parton (left) and particle (right) level.