

1 SEARCH FOR PRODUCTION OF A HIGGS BOSON AND A SINGLE TOP  
2 QUARK IN MULTILEPTON FINAL STATES IN  $pp$  COLLISIONS AT  $\sqrt{s} = 13$   
3 TeV.

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15 SEARCH FOR PRODUCTION OF A HIGGS BOSON AND A SINGLE TOP  
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18 Jose Andres Monroy Montañez, Ph.D.  
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21 Multivariate techniques are used to discriminate the signal from the dominant back-  
22 grounds. The analysis yields a 95% confidence level (C.L.) upper limit on the com-  
23 bined tH + ttH production cross section times branching ratio of 0.64 pb, with an  
24 expected limit of 0.32 pb, for a scenario with  $k_t = \pm 1.0$  and  $k_V = 1.0$ . Values of  $k_t$   
25 outside the range of  $\pm 1.25$  to  $\pm 1.60$  are excluded at 95% C.L., assuming  $k_V = 1.0$ .

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# <sup>323</sup> Chapter 1

## <sup>324</sup> Theoretical approach

### <sup>325</sup> 1.1 Introduction

<sup>326</sup> The physical description of the universe is a challenge that physicists have faced by  
<sup>327</sup> making theories that refine existing principles and proposing new ones in an attempt  
<sup>328</sup> to embrace emerging facts and phenomena.

<sup>329</sup> At the end of 1940s Julian Schwinger [1] and Richard P. Feynman [2], based on  
<sup>330</sup> the work of Sin-Itiro Tomonaga [3], developed an electromagnetic theory consistent  
<sup>331</sup> with special relativity and quantum mechanics that describes how matter and light  
<sup>332</sup> interact; the so-called *quantum electrodynamics* (QED) was born.

<sup>333</sup> QED has become the blueprint for developing theories that describe the universe.  
<sup>334</sup> It was the first example of a quantum field theory (QFT), which is the theoretical  
<sup>335</sup> framework for building quantum mechanical models that describes particles and their  
<sup>336</sup> interactions. QFT is composed of a set of mathematical tools that combines classical  
<sup>337</sup> fields, special relativity and quantum mechanics, while keeping the quantum point  
<sup>338</sup> particles and locality ideas.

<sup>339</sup> This chapter gives an overview of the standard model of particle physics, starting

340 with a description of the particles and their interactions, followed by a description of  
 341 the electroweak interaction, the Higgs boson and the associated production of Higgs  
 342 boson and a single top quark ( $tH$ ). The description contained in this chapter is based  
 343 on References [4–6].

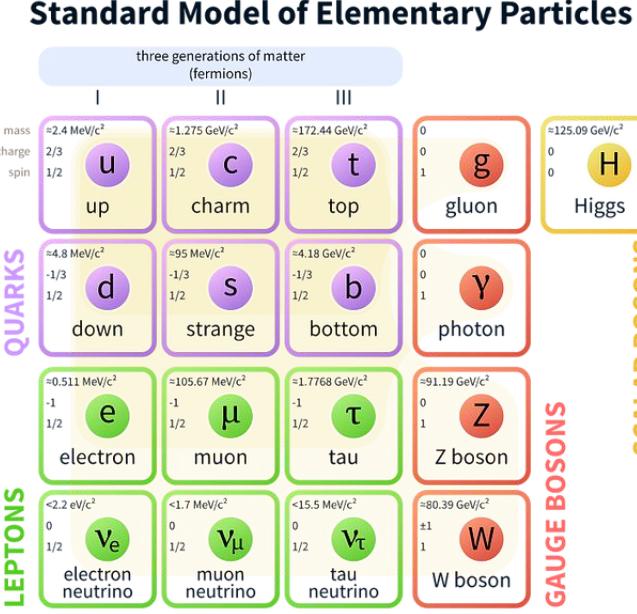
## 344 1.2 Standard model of particle physics

345 The *standard model of particle physics (SM)* describes particle physics at the funda-  
 346 mental level in terms of a collection of interacting particles and fields. The full picture  
 347 of the SM is composed of three fields<sup>1</sup> whose excitations are interpreted as particles  
 348 called mediators or force-carriers, a set of fields whose excitations are interpreted as  
 349 elementary particles interacting through the exchange of those mediators, and a field  
 350 that gives the mass to elementary particles. Figure 1.1 shows a scheme of the SM  
 351 particles’ organization. In addition, for each of the particles in the scheme there exists  
 352 an antiparticle with the same mass and opposite quantum numbers. The existence of  
 353 antiparticles is a prediction of the relativistic quantum mechanics from the solution  
 354 of the Dirac equation for which a negative energy solution is also possible. In some  
 355 cases a particle is its own anti-particle, like photon or Higgs boson.

356 The mathematical formulation of the SM is based on group theory and the use of  
 357 Noether’s theorem [8] which states that for a physical system modeled by a Lagrangian  
 358 that is invariant under a group of transformations a conservation law is expected. For  
 359 instance, a system described by a time-independent Lagrangian is invariant (symmet-  
 360 ric) under time changes (transformations) with the total energy conservation law as  
 361 the expected conservation law. In QED, the charge operator ( $Q$ ) is the generator of

---

<sup>1</sup> The formal and complete treatment of the SM is out of the scope of this document, however a plenty of textbooks describing it at several levels are available in the literature. The treatment in References [5, 6] is quite comprehensive and detailed. Note that gravitational field is not included in the standard model formulation



**Figure 1.1:** Schematic representation of the Standard Model of particle physics. The SM is a theoretical model intended to describe three of the four fundamental forces of the universe in terms of a set of particles and their interactions. [7].

362 the  $U(1)$  symmetry which according to the Noether's theorem means that there is a  
 363 conserved quantity; this conserved quantity is the electric charge and thus the law  
 364 conservation of electric charge is established.

365 In the SM, the symmetry group  $SU(3)_C \otimes SU(2)_L \otimes U(1)_Y$  describes three of the  
 366 four fundamental interactions in nature (see Section 1.2.2): strong interaction (SI),  
 367 weak interaction (WI) and electromagnetic interactions (EI) in terms of symmetries  
 368 associated to physical quantities:

- 369     • Strong:  $SU(3)_C$  associated to color charge
- 370     • Weak:  $SU(2)_L$  associated to weak isospin and chirality
- 371     • Electromagnetic:  $U(1)_Y$  associated to weak hypercharge and electric charge
- 372 It will be shown that the electromagnetic and weak interactions are combined in

373 the so-called electroweak interaction where chirality, hypercharge, weak isospin and  
 374 electric charge are the central concepts.

375 **1.2.1 Fermions**

376 The basic constituents of the ordinary matter at the lowest level, which form the set  
 377 of elementary particles in the SM formulation, are quarks and leptons. All of them  
 378 have spin 1/2, therefore they are classified as fermions since they obey Fermi-Dirac  
 379 statistics. There are six *flavors* of quarks and three of leptons organized in three  
 380 generations, or families, as shown in Table 1.1.

		Generation		
		1st	2nd	3rd
Leptons	Type	Electron (e)	Moun( $\mu$ )	Tau ( $\tau$ )
	Neutral	Electron neutrino ( $\nu_e$ )	Muon neutrino ( $\nu_\mu$ )	Tau neutrino ( $\nu_\tau$ )
Quarks	Up-type	Up (u)	Charm (c)	Top (t)
	Down-type	Down (d)	Strange (s)	Bottom (b)

**Table 1.1:** Fermions of the SM. There are six flavors of quarks and three of leptons, organized in three generations, or families, composed of two pairs of closely related particles. The close relationship is motivated by the fact that each pair of particles is a member of an  $SU(2)_L$  doublet that has an associated invariance under isospin transformations. WI between leptons is limited to the members of the same generation; WI between quarks is not limited but greatly favored, to same generation members.

381

382 There is a mass hierarchy between generations (see Table 1.2), where the higher  
 383 generation particles decays to the lower one, which can explain why the ordinary  
 384 matter is made of particles from the first generation. In the SM, neutrinos are modeled  
 385 as massless particles so they are not subject to this mass hierarchy; however, today it  
 386 is known that neutrinos are massive so the hierarchy could be restated. The reason  
 387 behind this mass hierarchy is one of the most important open questions in particle  
 388 physics, and it becomes more puzzling when noticing that the mass difference between

389 first and second generation fermions is small compared to the mass difference with  
 390 respect to the third generation.

Lepton	Mass (MeV/c <sup>2</sup> )	Quark	Mass (MeV/c <sup>2</sup> )
e	0.51	u	2.2
$\mu$	105.65	c	$1.28 \times 10^3$
$\tau$	1776.86	t	$173.1 \times 10^3$
$\nu_e$	Unknown	d	4.7
$\nu_\mu$	Unknown	s	96
$\tau_\mu$	Unknown	b	$4.18 \times 10^3$

**Table 1.2:** Fermion masses [9]. Generations differ by mass in a way that has been interpreted as a mass hierarchy. Approximate values with no uncertainties are used, for comparison purpose.

391

392        Usually, the second and third generation fermions are produced in high energy  
 393 processes, like the ones recreated in particle accelerators.

394 **1.2.1.1 Leptons**

395 A lepton is an elementary particle that is not subject to the SI. As seen in Table 1.1,  
 396 there are two types of leptons, the charged ones (electron, muon and tau) and the  
 397 neutral ones (the three neutrinos). The electric charge (Q) is the property that gives  
 398 leptons the ability to participate in the EI. From the classical point of view, Q plays  
 399 a central role determining, among others, the strength of the electric field through  
 400 which the electromagnetic force is exerted. It is clear that neutrinos are not affected  
 401 by EI because they don't carry electric charge.

402        Another feature of the leptons that is fundamental in the mathematical description  
 403 of the SM is the chirality, which is closely related to spin and helicity. Helicity  
 404 defines the handedness of a particle by relating its spin and momentum such that  
 405 if they are parallel then the particle is right-handed; if spin and momentum are

406 antiparallel the particle is said to be left-handed. The study of parity conservation  
 407 (or violation) in  $\beta$ -decay has shown that only left-handed electrons/neutrinos or right-  
 408 handed positrons/anti-neutrinos are created [10]; the inclusion of that feature in the  
 409 theory was achieved by using projection operators for helicity, however, helicity is  
 410 frame dependent for massive particles which makes it not Lorentz invariant and then  
 411 another related attribute has to be used: *chirality*.

412 Chirality is a purely quantum attribute which makes it not so easy to describe in  
 413 graphical terms but it defines how the wave function of a particle transforms under  
 414 certain rotations. As with helicity, there are two chiral states, left-handed chiral (L)  
 415 and right-handed chiral (R). In the highly relativistic limit where  $E \approx p \gg m$  helicity  
 416 and chirality converge, becoming exactly the same for massless particles.

417 In the following, when referring to left-handed (right-handed) it will mean left-  
 418 handed chiral (right-handed chiral). The fundamental fact about chirality is that  
 419 while EI and SI are not sensitive to chirality, in WI left-handed and right-handed  
 420 fermions are treated asymmetrically, such that only left-handed fermions and right-  
 421 handed anti-fermions are allowed to couple to WI mediators, which is a violation of  
 422 parity. The way to translate this statement in a formal mathematical formulation is  
 423 based on the isospin symmetry group  $SU(2)_L$ .

424 Each generation of leptons is seen as a weak isospin doublet.<sup>2</sup> The left-handed  
 425 charged lepton and its associated left-handed neutrino are arranged in doublets of  
 426 weak isospin  $T=1/2$  while their right-handed partners are singlets:

$$\begin{pmatrix} \nu_l \\ l \end{pmatrix}_L, l_R := \begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L, \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}_L, e_R, \mu_R, \tau_R, \nu_{eR}, \nu_{\mu R}, \nu_{\tau R} \quad (1.1)$$

427 The isospin third component refers to the eigenvalues of the weak isospin operator

---

<sup>2</sup> The weak isospin is an analogy of the isospin symmetry in strong interaction where neutron and proton are affected equally by strong force but differ in their charge.

428 which for doublets is  $T_3 = \pm 1/2$ , while for singlets it is  $T_3 = 0$ . The physical meaning  
 429 of this doublet-singlet arrangement falls in that the WI couples the two particles in  
 430 the doublet by exchanging the interaction mediator while the singlet member is not  
 431 involved in WI. The main properties of the leptons are summarized in Table 1.3.

432 Although all three flavor neutrinos have been observed, their masses remain un-  
 433 known and only some estimations have been made [11]. The main reason is that  
 434 the flavor eigenstates are not the same as the mass eigenstates which implies that  
 435 when a neutrino is created its mass state is a linear combination of the three mass  
 436 eigenstates and experiments can only probe the squared difference of the masses. The  
 437 Pontecorvo-Maki-Nakagawa-Sakata (PMNS) mixing matrix encodes the relationship  
 438 between flavor and mass eigenstates.

Lepton	$Q(e)$	$T_3$	$L_e$	$L_\mu$	$L_\tau$	Lifetime (s)
Electron (e)	-1	-1/2	1	0	0	Stable
Electron neutrino( $\nu_e$ )	0	1/2	1	0	0	Unknown
Muon ( $\mu$ )	-1	-1/2	0	1	0	$2.19 \times 10^{-6}$
Muon neutrino ( $\nu_\mu$ )	0	1/2	0	1	0	Unknown
Tau ( $\tau$ )	-1	-1/2	0	0	1	$290.3 \times 10^{-15}$
Tau neutrino ( $\nu_\tau$ )	0	1/2	0	0	1	Unknown

**Table 1.3:** Lepton properties [9]. Q: electric charge,  $T_3$ : weak isospin. Only left-handed leptons and right-handed anti-leptons participate in the WI. Anti-particles with inverted  $T_3$ , Q and lepton number complete the leptons set but are not listed. Right-handed leptons and left-handed anti-leptons, neither listed, form weak isospin singlets with  $T_3 = 0$  and do not take part in the weak interaction.

439

#### 440 1.2.1.2 Quarks

441 Quarks are the basic constituents of protons and neutrons. The way quarks join to  
 442 form bound states, called *hadrons*, is through the SI. Quarks are affected by all the  
 443 fundamental interactions which means that they carry all the four types of charges:  
 444 color, electric charge, weak isospin and mass.

Flavor	$Q(e)$	$I_3$	$T_3$	B	C	S	T	$B'$	Y	Color
Up (u)	2/3	1/2	1/2	1/3	0	0	0	0	1/3	r,b,g
Charm (c)	2/3	0	1/2	1/3	1	0	0	0	4/3	r,b,g
Top(t)	2/3	0	1/2	1/3	0	0	1	0	4/3	r,b,g
Down(d)	-1/3	-1/2	-1/2	1/3	0	0	0	0	1/3	r,b,g
Strange(s)	-1/3	0	-1/2	1/3	0	-1	0	0	-2/3	r,b,g
Bottom(b)	-1/3	0	-1/2	1/3	0	0	0	-1	-2/3	r,b,g

**Table 1.4:** Quark properties [9]. Q: electric charge,  $I_3$ : isospin,  $T_3$ : weak isospin, B: baryon number, C: charmness, S: strangeness, T: topness,  $B'$ : bottomness, Y: hypercharge. Anti-quarks posses the same mass and spin as quarks but all charges (color, flavor numbers) have opposite sign.

445

446 Table 1.4 summarizes the features of quarks, among which the most remarkable  
 447 is their fractional electric charge. Note that fractional charge is not a problem, given  
 448 that quarks are not found isolated, but serves to explain how composed particles are  
 449 formed out of two or more valence quarks<sup>3</sup>.

450 Color charge is responsible for the SI between quarks and is the symmetry ( $SU(3)_C$ )  
 451 that defines the formalism to describe SI. There are three colors: red (r), blue (b)  
 452 and green (g) and their corresponding three anti-colors; thus each quark carries one  
 453 color unit while anti-quarks carries one anti-color unit. As explained in Section 1.2.2,  
 454 quarks are not allowed to be isolated due to the color confinement effect, hence, their  
 455 features have been studied indirectly by observing their bound states created when

- 456 • one quark with a color charge is attracted by an anti-quark with the correspond-  
 457 ing anti-color charge forming a colorless particle called a *meson*.  
  
 458 • three quarks (anti-quarks) with different color (anti-color) charges are attracted  
 459 among them forming a colorless particle called a *baryon (anti-baryon)*.

---

<sup>3</sup> Hadrons can contain an indefinite number of virtual quarks and gluons, known as the quark and gluon sea, but only the valence quarks determine hadrons' quantum numbers.

460 In practice, when a quark is left alone isolated a process called *hadronization* occurs  
 461 where the quark emits gluons (see Section 1.2.4) which eventually will generate new  
 462 quark-antiquark pairs and so on; those quarks will recombine to form hadrons that  
 463 will decay into leptons. This proliferation of particles looks like a *jet* coming from  
 464 the isolated quark. More details about the hadronization process and jet structure  
 465 will be given in chapter3.

466 In the first version of the quark model (1964), M. Gell-Mann [12] and G. Zweig  
 467 [13, 14] developed a consistent way to classify hadrons according to their properties.  
 468 Only three quarks (u, d, s) were involved in a scheme in which all baryons have baryon  
 469 number  $B=1$  and therefore quarks have  $B=1/3$ ; non-baryons have  $B=0$ . Baryon  
 470 number is conserved in SI and EI which means that single quarks cannot be created  
 471 but in pairs  $q - \bar{q}$ .

472 The scheme organizes baryons in a two-dimensional space ( $I_3$  - Y); Y (hyper-  
 473 charge) and  $I_3$  (isospin) are quantum numbers related by the Gell-Mann-Nishijima  
 474 formula [15, 16]:

$$Q = I_3 + \frac{Y}{2} \quad (1.2)$$

475 where  $Y = B + S + C + T + B'$  are the quantum numbers listed in Table 1.4.

476 There are six quark flavors organized in three generations (see Table 1.1) fol-  
 477 lowing a mass hierarchy which, again, implies that higher generations decay to first  
 478 generation quarks.

	Quarks			$T_3$	$Y_W$	Leptons			$T_3$	$Y_W$
Doublets	$(\frac{u}{d'})_L$	$(\frac{c}{s'})_L$	$(\frac{t}{b'})_L$	$(\frac{1/2}{-1/2})$	$1/3$	$(\nu_e)_L$	$(\nu_\mu)_L$	$(\nu_\tau)_L$	$(\frac{1/2}{-1/2})$	-1
Singlets	$u_R$	$c_R$	$t_R$	0	$4/3$	$\nu_{eR}$	$\nu_{\mu R}$	$\nu_{\tau R}$		
	$d'_R$	$s'_R$	$b'_R$	0	$-2/3$	$e_R$	$\mu_R$	$\tau_R$	0	-2

**Table 1.5:** Fermion weak isospin and weak hypercharge multiplets. Weak hypercharge is calculated through the Gell-Mann-Nishijima formula 1.2 but using the weak isospin and charge for quarks.

479

480 Isospin doublets of quarks are also defined (see Table 1.5), and same as for neutrinos, the WI eigenstates are not the same as the mass eigenstates which means that  
 481 members of different quark generations are connected by the WI mediator; thus, up-type quarks are coupled not to down-type quarks (the mass eigenstates) directly but  
 482 to a superposition of down-type quarks ( $q'_d$ ; *the weak eigenstates*) via WI according  
 483 to:

486

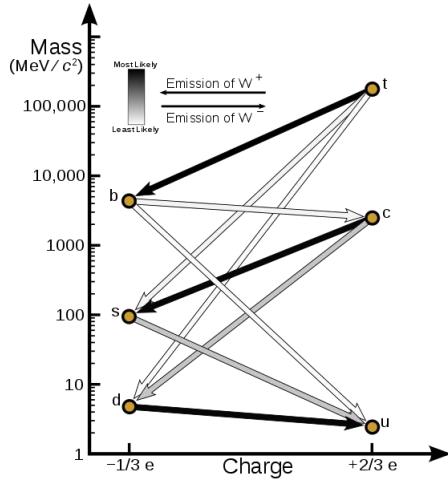
$$\begin{aligned} q'_d &= V_{CKM} q_d \\ \begin{pmatrix} d' \\ s' \\ b' \end{pmatrix} &= \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix} \end{aligned} \quad (1.3)$$

487 where  $V_{CKM}$  is known as Cabibbo-Kobayashi-Maskawa (CKM) mixing matrix [17,18]  
 488 given by

$$\begin{pmatrix} |V_{ud}| & |V_{us}| & |V_{ub}| \\ |V_{cd}| & |V_{cs}| & |V_{cb}| \\ |V_{td}| & |V_{ts}| & |V_{tb}| \end{pmatrix} = \begin{pmatrix} 0.97427 \pm 0.00015 & 0.22534 \pm 0.00065 & 0.00351^{+0.00015}_{-0.00014} \\ 0.22520 \pm 0.00065 & 0.97344 \pm 0.00016 & 0.0412^{+0.0011}_{-0.0005} \\ 0.00867^{+0.00029}_{-0.00031} & 0.0404^{+0.0011}_{-0.0005} & 0.999146^{+0.000021}_{-0.000046} \end{pmatrix}. \quad (1.4)$$

489 The weak decays of quarks are represented in the diagram of Figure 1.2; again  
 490 the CKM matrix plays a central role since it contains the probabilities for the different  
 491 quark decay channels, in particular, note that quark decays are greatly favored  
 492 between generation members.

493 CKM matrix is a  $3 \times 3$  unitary matrix parametrized by three mixing angles and  
 494 the *CP-mixing phase*; the latter is the parameter responsible for the Charge-Parity



**Figure 1.2:** Transformations between quarks through the exchange of a WI. Higher generations quarks decay to first generation quarks by emitting a W boson. The arrow color indicates the likelihood of the transition according to the grey scale in the top left side which represent the CKM matrix parameters [19].

495 symmetry violation (CP-violation) in the SM. The fact that the top quark decays  
 496 almost all the time to a bottom quark is exploited in this thesis when making the  
 497 selection of the signal events by requiring the presence of a jet tagged as a jet coming  
 498 from a  $b$  quark in the final state.

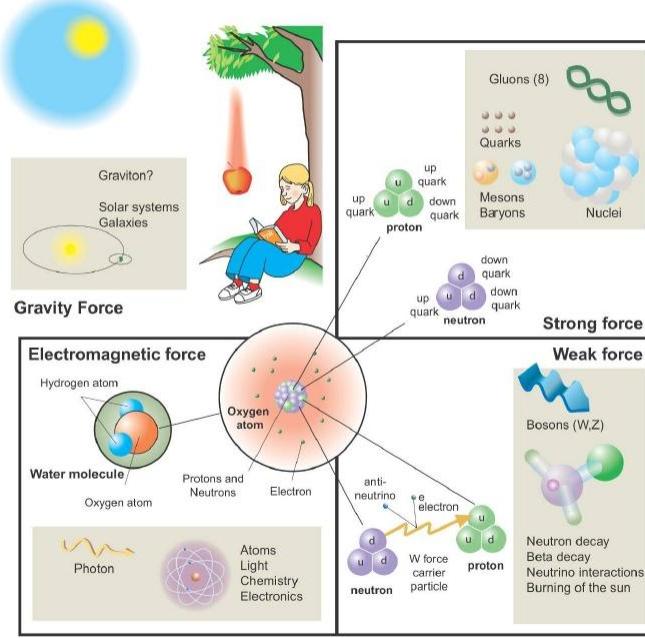
### 499 1.2.2 Fundamental interactions

500 Even though there are many manifestations of force in nature, like the ones repre-  
 501 sented in Figure 1.3, we can classify all of them in four fundamental interactions:

- 502 • *Electromagnetic interaction (EI)* affects particles that are *electrically charged*,  
 503 like electrons and protons. Figure 1.4a. shows a graphical representation, known  
 504 as *Feynman diagram*, of electron-electron scattering.
- 505 • *Strong interaction (SI)* described by Quantum Chromodynamics (QCD). Hadrons  
 506 like the proton and the neutron have internal structure given that they are com-

## Fundamental interactions.

Illustration: Typoform



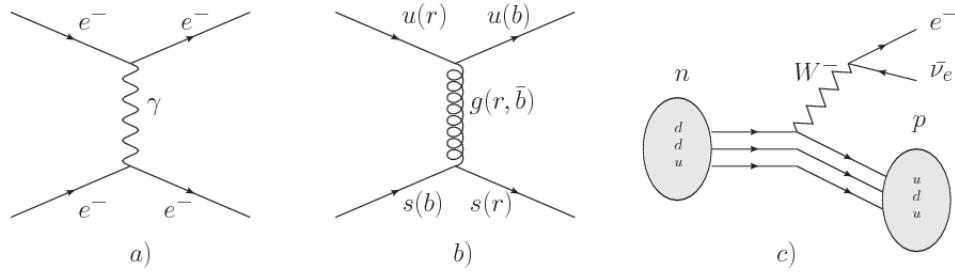
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**Figure 1.3:** Fundamental interactions in nature. Despite the many manifestations of forces in nature, we can track all of them back to one of the fundamental interactions. The most common forces are gravity and electromagnetic given that all of us are subject and experience them in everyday life.

507 posed of two or more valence quarks<sup>4</sup>. Quarks have fractional electric charge  
 508 which means that they are subject to electromagnetic interaction and in the case  
 509 of the proton they should break apart due to electrostatic repulsion; however,  
 510 quarks are held together inside the hadrons against their electrostatic repulsion  
 511 by the *Strong Force* through the exchange of *gluons*. The analog to the electric  
 512 charge is the *color charge*. Electrons and photons are elementary particles as  
 513 quarks but they don't carry color charge, therefore they are not subject to SI. A  
 514 Feynman diagram for gluon exchange between quarks is shown in Figure 1.4b.

- 515 • *Weak interaction (WI)* described by the weak theory (WT), is responsible, for  
 516 instance, for the radioactive decay in atoms and the deuterium production

<sup>4</sup> Particles made of four and five quarks are exotic states not so common.



**Figure 1.4:** Feynman diagrams representing the interactions in SM; a) EI:  $e$ - $e$  scattering; b) SI: gluon exchange between quarks ; c) WI:  $\beta$ -decay

within the sun. Quarks and leptons are the particles affected by the weak interaction; they possess a property called *flavor charge* (see 1.2.1) which can be changed by emitting or absorbing one weak force mediator. There are three mediators of the *weak force* known as  $Z$  boson in the case of electrically neutral flavor changes and  $W^\pm$  bosons in the case of electrically charged flavor changes. The *weak isospin* is the WI analog to electric charge in EI, and color charge in SI, and defines how quarks and leptons are affected by the weak force. Figure 1.4c. shows the Feynman diagram of  $\beta$ -decay where a neutron ( $n$ ) is transformed in a proton ( $p$ ) by emitting a  $W^-$  particle.

- *Gravitational interaction (GI)* described by General Theory of Relativity (GR). It is responsible for the structure of galaxies and black holes as well as the expansion of the universe. As a classical theory, in the sense that it can be formulated without even appeal to the concept of quantization, it implies that the space-time is a continuum and predictions can be made without limitation to the precision of the measurement tools. The latter represents a direct contradiction of the quantum mechanics principles. Gravity is deterministic while quantum mechanics is probabilistic; despite that, efforts to develop a quantum theory of gravity have predicted the *graviton* as mediator of the gravitational

535 force<sup>5</sup>.

Interaction	Acts on	Relative strength	Range (m)	Mediators
Electromagnetic (QED)	Electrically charged particles	$10^{-2}$	Infinite	Photon
Strong (QCD)	Quarks and gluons	1	$10^{-15}$	Gluon
Weak (WI)	Leptons and quarks	$10^{-6}$	$10^{-18}$	$W^\pm, Z$
Gravitational (GI)	Massive particles	$10^{-39}$	Infinite	Graviton

Table 1.6: Fundamental interactions features [20].

536

537 Table 1.6 summarizes the main features of the fundamental interactions. The  
 538 strength of the interactions is represented by the coupling constants which depend  
 539 on the energy scale at which the interaction is evaluated, therefore, it is the relative  
 540 strength of the fundamental forces that reveals the meaning of strong and weak; in  
 541 a context where the relative strength of the SI is 1, the EI is about hundred times  
 542 weaker and WI is about million times weaker than the SI. A good description on how  
 543 the relative strength and range of the fundamental interactions are calculated can  
 544 be found in References [20, 21]. In the everyday life, only EI and GI are explicitly  
 545 experienced due to the range of these interactions; i.e., at the human scale distances  
 546 only EI and GI have appreciable effects, in contrast to SI which at distances greater  
 547 than  $10^{-15}$ m become negligible. Is it important to clarify that the weakness of the  
 548 WI is attributed to the fact that its mediators are highly massive which affects the  
 549 propagators of the interaction, as a result, the effect of the coupling constant is  
 550 reduced.

---

<sup>5</sup> Actually a wide variety of theories have been developed in an attempt to describe gravity; some famous examples are string theory and supergravity.

551    **1.2.3    Gauge invariance.**

552    QED was built successfully on the basis of the classical electrodynamics theory (CED)  
 553    of Maxwell and Lorentz, following theoretical and experimental requirements imposed  
 554    by

- 555       • Lorentz invariance: independence on the reference frame.
- 556       • Locality: interacting fields are evaluated at the same space-time point to avoid  
 557              action at a distance.
- 558       • Renormalizability: physical predictions are finite and well defined.
- 559       • Particle spectrum, symmetries and conservation laws already known must emerge  
 560              from the theory.
- 561       • Local gauge invariance.

562       The gauge invariance requirement reflects the fact that the fundamental fields  
 563       cannot be directly measured but associated fields which are the observables. Electric  
 564       (**E**) and magnetic (**B**) fields in CED are associated with the electric scalar potential  
 565        $V$  and the vector potential **A**. In particular, **E** can be obtained by measuring the  
 566       change in the space of the scalar potential ( $\Delta V$ ); however, two scalar potentials  
 567       differing by a constant  $f$  correspond to the same electric field. The same happens  
 568       in the case of the vector potential **A**; thus, different configurations of the associated  
 569       fields result in the same set of values of the observables. The freedom in choosing one  
 570       particular configuration is known as *gauge freedom*; the transformation law connecting  
 571       two configurations is known as *gauge transformation* and the fact that the observables  
 572       are not affected by a gauge transformation is called *gauge invariance*.

573       When the gauge transformation:

$$\begin{aligned} \mathbf{A} &\rightarrow \mathbf{A} - \Delta f \\ V &\rightarrow V - \frac{\partial f}{\partial t} \end{aligned} \tag{1.5}$$

574 is applied to Maxwell equations, they are still satisfied and the fields remain invariant.  
 575 Thus, CED is invariant under gauge transformations and is called a *gauge theory*.  
 576 The set of all gauge transformations form the *symmetry group* of the theory, which  
 577 according to the group theory, has a set of *group generators*. The number of group  
 578 generators determine the number of *gauge fields* of the theory.

579 As mentioned in the first lines of Section 1.2, QED has one symmetry group ( $U(1)$ )  
 580 with one group generator (the  $Q$  operator) and one gauge field (the electromagnetic  
 581 field  $A^\mu$ ). In CED there is not a clear definition, beyond the historical convention,  
 582 of which fields are the fundamental and which are the associated, but in QED the  
 583 fundamental field is  $A^\mu$ . When a gauge theory is quantized, the gauge fields are  
 584 quantized and their quanta are called *gauge bosons*. The word boson characterizes  
 585 particles with integer spin which obey Bose-Einstein statistics.

586 As will be detailed in Section 1.3, interactions between particles in a system can  
 587 be obtained by considering first the Lagrangian density of free particles in the sys-  
 588 tem, which of course is incomplete because the interaction terms have been left out,  
 589 and demanding global phase transformation invariance. Global phase transforma-  
 590 tion means that a gauge transformation is performed identically to every point  
 591 in the space<sup>6</sup> and the Lagrangian remains invariant. Then, the global transforma-  
 592 tion is promoted to a local phase transformation (this time the gauge transforma-  
 593 tion depends on the position in space) and again invariance is required.

---

<sup>6</sup> Here space corresponds to the 4-dimensional space i.e. space-time.

594 Due to the space dependence of the local transformation, the Lagrangian density is  
 595 not invariant anymore. In order to reinstate the gauge invariance, the gauge covariant  
 596 derivative is introduced in the Lagrangian and with it the gauge field responsible for  
 597 the interaction between particles in the system. The new Lagrangian density is gauge  
 598 invariant, includes the interaction terms needed to account for the interactions and  
 599 provides a way to explain the interaction between particles through the exchange of  
 600 the gauge boson.

601 This recipe was used to build QED and the theories that aim to explain the  
 602 fundamental interactions.

### 603 1.2.4 Gauge bosons

604 The importance of the gauge bosons comes from the fact that they are the force  
 605 mediators or force carriers. The features of the gauge bosons reflect those of the fields  
 606 they represent and they are extracted from the Lagrangian density used to describe  
 607 the interactions. In Section 1.3, it will be shown how the gauge bosons of the EI and  
 608 WI emerge from the electroweak Lagrangian. The SI gauge bosons features are also  
 609 extracted from the SI Lagrangian but it is not detailed in this document. The main  
 610 features of the SM gauge bosons will be briefly presented below and summarized in  
 611 Table 1.7.

- 612 • **Photon.** EI occurs when the photon couples to (is exchanged between) parti-  
 613 cles carrying electric charge; however, The photon itself does not carry electric  
 614 charge, therefore, there is no coupling between photons. Given that the photon  
 615 is massless the EI is of infinite range, i.e., electrically charged particles interact  
 616 even if they are located far away one from each other; this also implies that  
 617 photons always move with the speed of light.

- 618     • **Gluon.** SI is mediated by gluons which just as photons are massless. They  
 619       carry one unit of color charge and one unit of anticolor charge, hence, gluons  
 620       can couple to other gluons. As a result, the range of the SI is not infinite  
 621       but very short due to the attraction between gluons, giving rise to the *color*  
 622       *confinement* which explains why color charged particles cannot be isolated but  
 623       live within composite particles, like quarks inside protons.
- 624     • **W, Z.**  $W^\pm$  and Z, are massive which explains their short-range. Given that  
 625       the WI is the only interaction that can change the flavor of the interacting  
 626       particles, the W boson is the responsible for the nuclear transmutation where  
 627       a neutron is converted into a proton or vice versa with the involvement of an  
 628       electron and a neutrino (see Figure 1.4c). The Z boson is the responsible for the  
 629       neutral weak processes like neutrino elastic scattering where no electric charge  
 630       but momentum transference is involved. WI gauge bosons carry isospin charge  
 631       which makes interaction between them possible.

Interaction	Mediator	Electric charge (e)	Color charge	Weak Isospin	mass (GeV/c <sup>2</sup> )
Electromagnetic	Photon ( $\gamma$ )	0	No	0	0
Strong	Gluon (g)	0	Yes -octet	No	0
Weak	$W^\pm$	$\pm 1$	No	$\pm 1$	$80.385 \pm 0.015$
	Z	0	No	0	$91.188 \pm 0.002$

**Table 1.7:** SM gauge bosons main features [9].

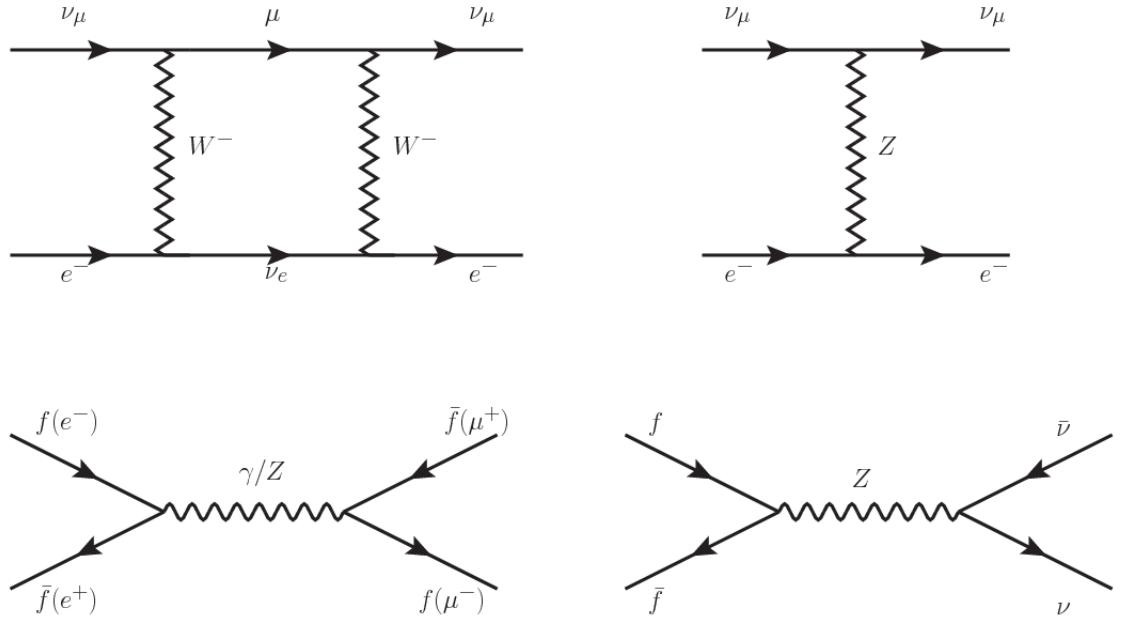
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633     

### 1.3 Electroweak unification and the Higgs 634                   mechanism

635     Physicists dream of building a theory that contains all the interactions in one single  
 636       interaction, i.e., showing that at some scale in energy all the four fundamental inter-

actions are unified and only one interaction emerges in a *Theory of everything*. The first sign of the feasibility of such unification came from success in the construction of the CED. Einstein spent years trying to reach that full unification, which by 1920 only involved electromagnetism and gravity, with no success; however, a new partial unification was achieved in the 1960's, when S.Glashow [22], A.Salam [23] and S.Weinberg [24] independently proposed that electromagnetic and weak interactions are two manifestations of a more general interaction called *electroweak interaction* (EWI). EWI was developed by following the useful prescription provided by QED and the gauge invariance principles.



**Figure 1.5:** Top:  $\nu_\mu - e^-$  scattering going through charged currents (left) and neutral currents (right). Bottom: neutral current processes for charged fermions (left) and involving neutrinos (right). While neutral current processes involving only charged fermions can proceed through EI or WI, those involving neutrinos can only proceed via WI.

The *classic* weak theory developed by Fermi, did not have the concept of the W boson but instead it was treated as a point interaction with the dimensionful constant  $G_F$  associated with it. It works really well at low energies very far off the W mass

649 shell. When going up in energy, the theory of weak interactions involving the W  
 650 boson is capable of explaining the  $\beta$ -decay and in general the processes mediated by  
 651  $W^\pm$  bosons. However, there were some processes like the  $\nu_\mu - e$  scattering which  
 652 would require the exchange of two W bosons (see Figure 1.5 top diagrams) giving  
 653 rise to divergent loop integrals and then non-finite predictions. The EWI theory, by  
 654 including neutral currents involving fermions via the exchange of a neutral bosons Z,  
 655 overcomes those divergences and the predictions become realistic.

656       Neutral weak interaction vertices conserve flavor in the same way as the electro-  
 657 magnetic vertices do, but additionally, the Z boson can couple to neutrinos which  
 658 implies that processes involving charged fermions can proceed through EI or WI but  
 659 processes involving neutrinos can proceed only through WI.

660       The prescription to build a gauge theory of the WI consists of proposing a free  
 661 field Lagrangian density that includes the particles involved; next, by requesting  
 662 invariance under global phase transformations first and generalizing to local phase  
 663 transformations invariance later, the conserved currents are identified and interactions  
 664 are generated by introducing gauge fields. Given that the goal is to include the EI  
 665 and WI in a single theory, the group symmetry considered should be a combination of  
 666  $SU(2)_L$  and  $U(1)_{em}$ , however the latter cannot be used directly because the EI treats  
 667 left and right-handed particles indistinctly in contrast to the former. Fortunately, the  
 668 weak hypercharge, which is a combination of the weak isospin and the electric charge  
 669 (Eqn. 1.2) is suitable to be used since it is conserved by the EI and WI. Thus, the  
 670 symmetry group to be considered is

$$G \equiv SU(2)_L \otimes U(1)_Y \quad (1.6)$$

671       The following treatment applies to any of the fermion generations, but for sim-

672 plicity the first generation of leptons will be considered [5, 6, 25, 26].

673 Given the first generation of leptons

$$\psi_1 = \begin{pmatrix} \nu_e \\ e^- \end{pmatrix}_L, \quad \psi_2 = \nu_{eR}, \quad \psi_3 = e_R^- \quad (1.7)$$

674 the charged fermionic currents are given by

$$J_\mu \equiv J_\mu^+ = \bar{\nu}_{eL} \gamma_\mu e_L, \quad J_\mu^\dagger \equiv J_\mu^- = \bar{e}_L \gamma_\mu \nu_{eL} \quad (1.8)$$

675 and the free Lagrangian is given by

$$\mathcal{L}_0 = \sum_{j=1}^3 i\bar{\psi}_j(x) \gamma^\mu \partial_\mu \psi_j(x). \quad (1.9)$$

676 Mass terms are included directly in the QED free Lagrangians since they preserve  
 677 the invariance under the symmetry transformations involved which treat left and right  
 678 handed particles similarly, however mass terms of the form

$$m_W^2 W_\mu^\dagger(x) W^\mu(x) + \frac{1}{2} m_Z^2 Z_\mu(x) Z^\mu(x) - m_e \bar{\psi}_e(x) \psi_e(x) \quad (1.10)$$

679 which represent the mass of  $W^\pm$ , Z and electrons, are not invariant under G trans-  
 680 formations, therefore the gauge fields described by the EWI are in principle massless.

681 Experiments have shown that the EWI gauge fields are not massless [27–30];  
 682 however, they have to acquire mass through a mechanism compatible with the gauge  
 683 invariance; that mechanism is known as the *Higgs mechanism* and will be considered  
 684 later in this Section. The global transformations in the combined symmetry group G  
 685 can be written as

$$\begin{aligned}
\psi_1(x) &\xrightarrow{G} \psi'_1(x) \equiv U_Y U_L \psi_1(x), \\
\psi_2(x) &\xrightarrow{G} \psi'_2(x) \equiv U_Y \psi_2(x), \\
\psi_3(x) &\xrightarrow{G} \psi'_3(x) \equiv U_Y \psi_3(x)
\end{aligned} \tag{1.11}$$

686 where  $U_L$  represent the  $SU(2)_L$  transformation acting only on the weak isospin dou-  
 687 blet and  $U_Y$  represent the  $U(1)_Y$  transformation acting on all the weak isospin mul-  
 688 tiplets. Explicitly

$$U_L \equiv \exp\left(i \frac{\sigma_i}{2} \alpha^i\right), \quad U_Y \equiv \exp(i y_i \beta) \quad (i = 1, 2, 3) \tag{1.12}$$

689 with  $\sigma_i$  the Pauli matrices and  $y_i$  the weak hypercharges. In order to promote the  
 690 transformations from global to local while keeping the invariance, it is required that  
 691  $\alpha^i = \alpha^i(x)$ ,  $\beta = \beta(x)$  and the replacement of the ordinary derivatives by the covariant  
 692 derivatives

$$\begin{aligned}
D_\mu \psi_1(x) &\equiv \left[ \partial_\mu + ig\sigma_i W_\mu^i(x)/2 + ig'y_1 B_\mu(x) \right] \psi_1(x) \\
D_\mu \psi_2(x) &\equiv \left[ \partial_\mu + ig'y_2 B_\mu(x) \right] \psi_2(x) \\
D_\mu \psi_3(x) &\equiv \left[ \partial_\mu + ig'y_3 B_\mu(x) \right] \psi_3(x)
\end{aligned} \tag{1.13}$$

693 introducing in this way four gauge fields,  $W_\mu^i(x)$  and  $B_\mu(x)$ , in the process. The  
 694 covariant derivatives (Eqn. 1.13) are required to transform in the same way as fermion  
 695 fields  $\psi_i(x)$  themselves, therefore, the gauge fields transform as:

$$\begin{aligned} B_\mu(x) &\xrightarrow{G} B'_\mu(x) \equiv B_\mu(x) - \frac{1}{g'} \partial_\mu \beta(x) \\ W_\mu^i(x) &\xrightarrow{G} W_\mu^{i\prime}(x) \equiv W_\mu^i(x) - \frac{i}{g} \partial_\mu \alpha_i(x) - \varepsilon_{ijk} \alpha_i(x) W_\mu^j(x). \end{aligned} \quad (1.14)$$

696 The G invariant version of the Lagrangian density 1.9 can be written as

$$\mathcal{L}_0 = \sum_{j=1}^3 i \bar{\psi}_j(x) \gamma^\mu D_\mu \psi_j(x) \quad (1.15)$$

697 where free massless fermion and gauge fields and fermion-gauge boson interactions  
698 are included. The EWI Lagrangian density must additionally include kinetic terms  
699 for the gauge fields ( $\mathcal{L}_G$ ) which are built from the field strengths, according to

$$B_{\mu\nu}(x) \equiv \partial_\mu B_\nu - \partial_\nu B_\mu \quad (1.16)$$

$$W_{\mu\nu}^i(x) \equiv \partial_\mu W_\nu^i(x) - \partial_\nu W_\mu^i(x) - g \varepsilon^{ijk} W_\mu^j W_\nu^k \quad (1.17)$$

700 the last term in Eqn. 1.17 is added in order to hold the gauge invariance; therefore,

$$\mathcal{L}_G = -\frac{1}{4} B_{\mu\nu}(x) B^{\mu\nu}(x) - \frac{1}{4} W_{\mu\nu}^i(x) W_i^{\mu\nu}(x) \quad (1.18)$$

701 which contains not only the free gauge fields contributions, but also the gauge fields  
702 self-interactions and interactions among them.

703 The three weak isospin conserved currents resulting from the  $SU(2)_L$  symmetry  
704 are given by

$$J_\mu^i(x) = \frac{1}{2} \bar{\psi}_1(x) \gamma_\mu \sigma^i \psi_1(x) \quad (1.19)$$

705 while the weak hypercharge conserved current resulting from the  $U(1)_Y$  symmetry is  
 706 given by

$$J_\mu^Y = \sum_{j=1}^3 \bar{\psi}_j(x) \gamma_\mu y_j \psi_j(x) \quad (1.20)$$

707 In order to evaluate the electroweak interactions modeled by an isos triplet field  
 708  $W_\mu^i$  that couples to isospin currents  $J_\mu^i$  with strength  $g$  and additionally the singlet  
 709 field  $B_\mu$  which couples to the weak hypercharge current  $J_\mu^Y$  with strength  $g'/2$ . The  
 710 interaction Lagrangian density to be considered is

$$\mathcal{L}_I = -g J^{i\mu}(x) W_\mu^i(x) - \frac{g'}{2} J^{Y\mu}(x) B_\mu(x) \quad (1.21)$$

711 Note that the weak isospin currents are not the same as the charged fermionic cur-  
 712 rents that were used to describe the WI (Eqn. 1.8), since the weak isospin eigenstates  
 713 are not the same as the mass eigenstates, but they are closely related

$$J_\mu = \frac{1}{2}(J_\mu^1 + iJ_\mu^2), \quad J_\mu^\dagger = \frac{1}{2}(J_\mu^1 - iJ_\mu^2). \quad (1.22)$$

714 The same happens with the gauge fields  $W_\mu^i$  which are related to the mass eigen-  
 715 states  $W^\pm$  by

$$W_\mu^+ = \frac{1}{\sqrt{2}}(W_\mu^1 - iW_\mu^2), \quad W_\mu^- = \frac{1}{\sqrt{2}}(W_\mu^1 + iW_\mu^2). \quad (1.23)$$

716 The fact that there are three weak isospin conserved currents is an indication that  
 717 in addition to the charged fermionic currents, which couple charged to neutral leptons,  
 718 there should be a neutral fermionic current that does not involve electric charge  
 719 exchange; therefore, it couples neutral fermions or fermions of the same electric charge.  
 720 The third weak isospin current contains a term that is similar to the electromagnetic

721 current ( $j_\mu^{em}$ ), indicating that there is a relation between them and resembling the  
 722 Gell-Mann-Nishijima formula 1.2 adapted to electroweak interactions

$$Q = T_3 + \frac{Y_W}{2}. \quad (1.24)$$

723 Just as  $Q$  generates the  $U(1)_{em}$  symmetry, the weak hypercharge generates the  
 724  $U(1)_Y$  symmetry as said before. It is possible to write the relationship in terms of  
 725 the currents as

$$j_\mu^{em} = J_\mu^3 + \frac{1}{2} J_\mu^Y. \quad (1.25)$$

726 The neutral gauge fields  $W_\mu^3$  and  $B_\mu$  cannot be directly identified with the  $Z$   
 727 and the photon fields since the photon interacts similarly with left and right-handed  
 728 fermions; however, they are related through a linear combination given by

$$\begin{aligned} A_\mu &= B_\mu \cos \theta_W + W_\mu^3 \sin \theta_W \\ Z_\mu &= -B_\mu \sin \theta_W + W_\mu^3 \cos \theta_W \end{aligned} \quad (1.26)$$

where  $\theta_W$  is known as the *Weinberg angle*. The interaction Lagrangian is now given by

$$\begin{aligned} \mathcal{L}_I = -\frac{g}{\sqrt{2}}(J^\mu W_\mu^+ + J^{\mu\dagger} W_\mu^-) - &\left(g \sin \theta_W J_\mu^3 + g' \cos \theta_W \frac{J_\mu^Y}{2}\right) A^\mu \\ &- \left(g \cos \theta_W J_\mu^3 - g' \sin \theta_W \frac{J_\mu^Y}{2}\right) Z^\mu \end{aligned} \quad (1.27)$$

729 the first term is the weak charged current interaction, while the second term is the

730 electromagnetic interaction under the condition

$$g \sin \theta_W = g' \cos \theta_W = e, \quad \frac{g'}{g} = \tan \theta_W \quad (1.28)$$

731 contained in the Eqn.1.25; the third term is the neutral weak current.

732

733 Note that the neutral fields transformation given by the Eqn. 1.26 can be written  
 734 in terms of the coupling constants  $g$  and  $g'$  as:

$$A_\mu = \frac{g' W_\mu^3 + g B_\mu}{\sqrt{g^2 + g'^2}}, \quad Z_\mu = \frac{g W_\mu^3 - g' B_\mu}{\sqrt{g^2 + g'^2}}. \quad (1.29)$$

735 So far, the Lagrangian density describing the non-massive EWI is:

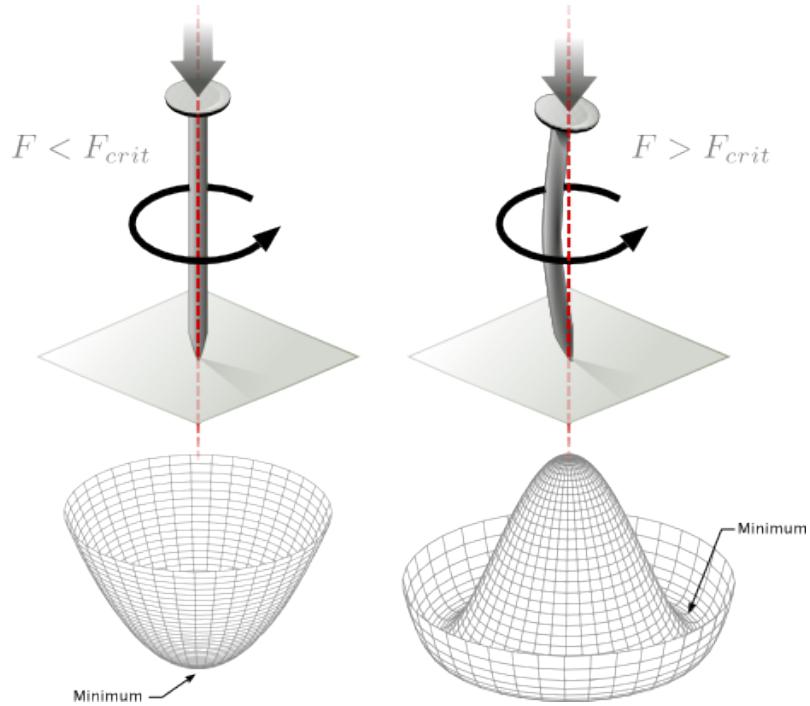
$$\mathcal{L}_{nmEWI} = \mathcal{L}_0 + \mathcal{L}_G \quad (1.30)$$

736 where fermion and gauge fields have been considered massless because their regular  
 737 mass terms are manifestly non invariant under  $G$  transformations; therefore, masses  
 738 have to be generated in a gauge invariant way. The mechanism by which this goal is  
 739 achieved is known as the *Higgs mechanism* and is closely connected to the concept of  
 740 *spontaneous symmetry breaking*.

### 741 1.3.1 Spontaneous symmetry breaking (SSB)

742 Figure 1.6 left shows a steel nail (top) which is subject to an external force; the form  
 743 of the potential energy is also shown (bottom).

744 Before reaching the critical force value, the system has rotational symmetry with  
 745 respect to the nail axis; however, after the critical force value is reached the nail buck-



**Figure 1.6:** Spontaneous symmetry breaking mechanism. The steel nail, subject to an external force (top left), has rotational symmetry with respect to its axis. When the external force overcomes a critical value the nail buckles (top right) choosing a minimal energy state (ground state) and thus *breaking spontaneously the rotational symmetry*. The potential energy (bottom) changes but holds the rotational symmetry; however, an infinite number of asymmetric ground states are generated and circularly distributed in the bottom of the potential [31].

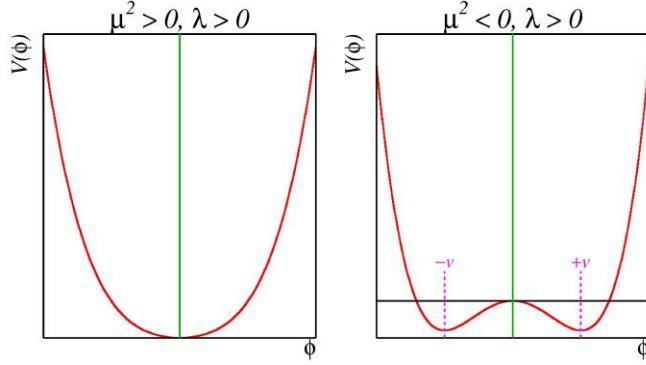
746 les (top right). The form of the potential energy (bottom right) changes appearing a  
 747 set of infinity minima but preserving its rotational symmetry. Right before the nail  
 748 buckles there is no indication of the direction the nail will bend because any of the  
 749 directions are equivalent, but once the nail bends, choosing a direction, an arbitrary  
 750 minimal energy state (ground state) is selected and it does not share the system's  
 751 rotational symmetry. This mechanism for reaching an asymmetric ground state is  
 752 known as *spontaneous symmetry breaking*.

753 The lesson from this analysis is that the way to introduce the SSB mechanism  
 754 into a system is by adding the appropriate potential to it.

755 Figure 1.7 shows a plot of the potential  $V(\phi)$  in the case of a scalar field  $\phi$

$$V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2 \quad (1.31)$$

If  $\mu^2 > 0$  the potential has only one minimum at  $\phi = 0$  and describes a scalar field with mass  $\mu$ . If  $\mu^2 < 0$  the potential has a local maximum at  $\phi = 0$  and two minima at  $\phi = \pm\sqrt{-\mu^2/\lambda}$  which enables the SSB mechanism to work.



**Figure 1.7:** Shape of the potential  $V(\phi)$  for  $\lambda > 0$  and:  $\mu^2 > 0$  (left) and  $\mu^2 < 0$  (right). The case  $\mu^2 < 0$  corresponds to the potential suitable for introducing the SSB mechanism by choosing one of the two ground states which are connected via reflection symmetry. [31].

In the case of a complex scalar field  $\phi(x)$

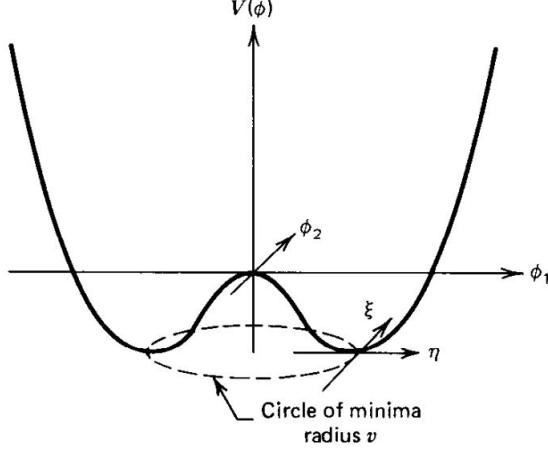
$$\phi(x) = \frac{1}{\sqrt{2}}(\phi_1 + i\phi_2) \quad (1.32)$$

the Lagrangian (invariant under global  $U(1)$  transformations) is given by

$$\mathcal{L} = (\partial_\mu \phi)^\dagger (\partial^\mu \phi) - V(\phi), \quad V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2 \quad (1.33)$$

where an appropriate potential has been added in order to introduce the SSB.

As seen in Figure 1.8, the potential has now an infinite number of minima circularly distributed along the  $\xi$ -direction which makes possible the occurrence of the SSB by choosing an arbitrary ground state; for instance,  $\xi = 0$ , i.e.  $\phi_1 = v, \phi_2 = 0$



**Figure 1.8:** Potential for complex scalar field. There is a circle of minima of radius  $v$  along the  $\xi$ -direction [6].

$$\phi_0 = \frac{v}{\sqrt{2}} \exp(i\xi) \quad \xrightarrow{\text{SSB}} \quad \phi_0 = \frac{v}{\sqrt{2}} \quad (1.34)$$

765 As usual, excitations over the ground state are studied by making an expansion  
766 about it; thus, the excitations can be parametrized as:

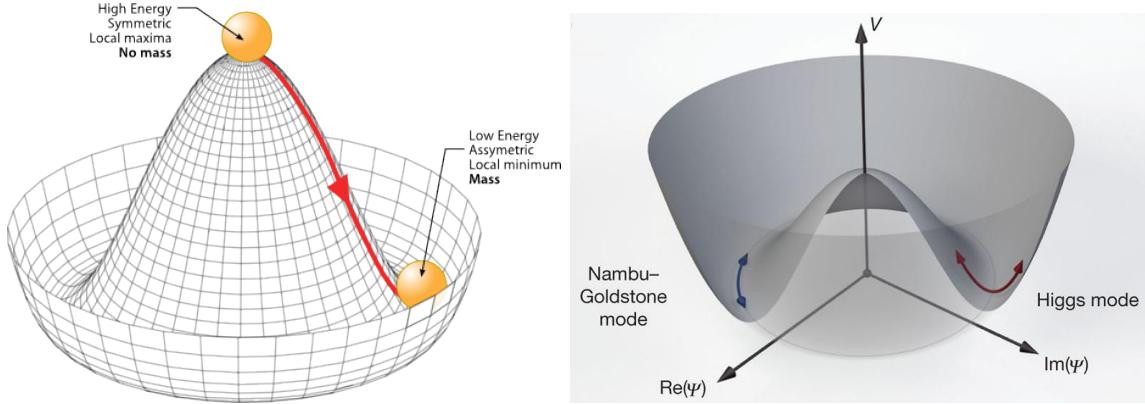
$$\phi(x) = \frac{1}{\sqrt{2}}(v + \eta(x) + i\xi(x)) \quad (1.35)$$

767 which when substituted into Eqn. 1.33 produces a Lagrangian in terms of the new  
768 fields  $\eta$  and  $\xi$

$$\mathcal{L}' = \frac{1}{2}(\partial_\mu \xi)^2 + \frac{1}{2}(\partial_\mu \eta)^2 + \mu^2 \eta^2 - V(\phi_0) - \lambda v \eta (\eta^2 + \xi^2) - \frac{\lambda}{4}(\eta^2 + \xi^2)^2 \quad (1.36)$$

769 where the last two terms represent the interactions and self-interaction between the  
770 two fields  $\eta$  and  $\xi$ . The particular feature of the SSB mechanism is revealed when  
771 looking to the first three terms of  $\mathcal{L}'$ . Before the SSB, only the massless  $\phi$  field is

772 present in the system; after the SSB there are two fields of which the  $\eta$ -field has  
 773 acquired mass  $m_\eta = \sqrt{-2\mu^2}$  while the  $\xi$ -field is still massless (see Figure 1.9).



**Figure 1.9:** SSB mechanism for a complex scalar field [31, 32].

774 Thus, the SSB mechanism serves as a method to generate mass but as a side effect  
 775 a massless field is introduced in the system. This fact is known as the Goldstone  
 776 theorem and states that a massless scalar field appears in the system for each con-  
 777 tinuous symmetry spontaneously broken. Another version of the Goldstone theorem  
 778 states that “if a Lagrangian is invariant under a continuous symmetry group  $G$ , but  
 779 the vacuum is only invariant under a subgroup  $H \subset G$ , then there must exist as many  
 780 massless spin-0 particles (Nambu-Goldstone bosons) as broken generators.” [26] The  
 781 Nambu-Goldstone boson can be understood considering that the potential in the  $\xi$ -  
 782 direction is flat so excitations in that direction are not energy consuming and thus  
 783 represent a massless state.

### 784 1.3.2 Higgs mechanism

785 When the SSB mechanism is introduced in the formulation of the EWI in an attempt  
 786 to generate the mass of the so far massless gauge bosons and fermions, an interesting  
 787 effect is revealed. In order to keep the  $G$  symmetry group invariance and generate

788 the mass of the EW gauge bosons, a G invariant Lagrangian density ( $\mathcal{L}_S$ ) has to be  
 789 added to the non massive EWI Lagrangian (Eqn. 1.30)

$$\mathcal{L}_S = (D_\mu \phi)^\dagger (D^\mu \phi) - \mu^2 \phi^\dagger \phi - \lambda (\phi^\dagger \phi)^2, \quad \lambda > 0, \mu^2 < 0 \quad (1.37)$$

$$D_\mu \phi = \left( i\partial_\mu - g \frac{\sigma_i}{2} W_\mu^i - g' \frac{Y}{2} B_\mu \right) \phi \quad (1.38)$$

790  $\phi$  has to be an isospin doublet of complex scalar fields so it preserves the G invariance;  
 791 thus  $\phi$  can be defined as:

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix}. \quad (1.39)$$

792 The minima of the potential are defined by

$$\phi^\dagger \phi = \frac{1}{2} (\phi_1^2 + \phi_2^2 + \phi_3^2 + \phi_4^2) = -\frac{\mu^2}{2\lambda}. \quad (1.40)$$

793 The choice of the ground state is critical. By choosing a ground state, invariant  
 794 under  $U(1)_{em}$  gauge symmetry, the photon will remain massless and the  $W^\pm$  and  $Z$   
 795 bosons masses will be generated which is exactly what is needed. In that sense, the  
 796 best choice corresponds to a weak isospin doublet with  $T_3 = -1/2$ ,  $Y_W = 1$  and  $Q = 0$   
 797 which defines a ground state with  $\phi_1 = \phi_2 = \phi_4$  and  $\phi_3 = v$ :

$$\phi_0 \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}, \quad v^2 \equiv -\frac{\mu^2}{\lambda}. \quad (1.41)$$

798 where the vacuum expectation value  $v$  is fixed by the Fermi coupling  $G_F$  according  
 799 to  $v = (\sqrt{2}G_F)^{1/2} \approx 246$  GeV.

800 The G symmetry has been broken and three Nambu-Goldstone bosons will appear.

801 The next step is to expand  $\phi$  about the chosen ground state as:

$$\phi(x) = \frac{1}{\sqrt{2}} \exp\left(\frac{i}{v} \sigma_i \theta^i(x)\right) \begin{pmatrix} 0 \\ v + H(x) \end{pmatrix} \approx \frac{1}{\sqrt{2}} \begin{pmatrix} \theta_1(x) + i\theta_2(x) \\ v + H(x) - i\theta_3(x) \end{pmatrix} \quad (1.42)$$

802 to describe fluctuations from the ground state  $\phi_0$ . The fields  $\theta_i(x)$  represent the  
 803 Nambu-Goldstone bosons while  $H(x)$  is known as *Higgs field*. The fundamental fea-  
 804 ture of the parametrization used is that the dependence on the  $\theta_i(x)$  fields is factored  
 805 out in a global phase that can be eliminated by taking the physical *unitary gauge*  
 806  $\theta_i(x) = 0$ . Therefore the expansion about the ground state is given by:

$$\phi(x) \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + H(x) \end{pmatrix} \quad (1.43)$$

807 which when substituted into  $\mathcal{L}_S$  (Eqn. 1.37) results in a Lagrangian containing the  
 808 now massive three gauge bosons  $W^\pm, Z$ , one massless gauge boson (photon) and  
 809 the new Higgs field ( $H$ ). The three degrees of freedom corresponding to the Nambu-  
 810 Goldstone bosons are now integrated into the massive gauge bosons as their lon-  
 811 gitudinal polarizations which were not available when they were massless particles.  
 812 The effect by which vector boson fields acquire mass after an spontaneous symmetry  
 813 breaking, but without an explicit gauge invariance breaking is known as the *Higgs*  
 814 *mechanism*.

815 The mechanism was proposed by three independent groups: F.Englert and R.Brout  
 816 in August 1964 [33], P.Higgs in October 1964 [34] and G.Guralnik, C.Hagen and  
 817 T.Kibble in November 1964 [35]; however, its importance was not realized until  
 818 S.Glashow [22], A.Salam [23] and S.Weinberg [24], independently, proposed that elec-  
 819 tromagnetic and weak interactions are two manifestations of a more general interac-  
 820 tion called *electroweak interaction* in 1967.

821 **1.3.3 Masses of the gauge bosons**

822 The masses of the gauge bosons are extracted by evaluating the kinetic part of La-  
 823 grangian  $\mathcal{L}_S$  in the ground state (known also as the vacuum expectation value), i.e.,

$$\left| \left( \partial_\mu - ig \frac{\sigma_i}{2} W_\mu^i - i \frac{g'}{2} B_\mu \right) \phi_0 \right|^2 = \left( \frac{1}{2} v g \right)^2 W_\mu^+ W^{-\mu} + \frac{1}{8} v^2 (W_\mu^3, B_\mu) \begin{pmatrix} g^2 & -gg' \\ -gg' & g'^2 \end{pmatrix} \begin{pmatrix} W^{3\mu} \\ B^\mu \end{pmatrix} \quad (1.44)$$

824 comparing with the typical mass term for a charged boson  $M_W^2 W^+ W^-$

$$M_W = \frac{1}{2} v g. \quad (1.45)$$

The second term in the right side of the Eqn.1.44 comprises the masses of the neutral bosons, but it needs to be written in terms of the gauge fields  $Z_\mu$  and  $A_\mu$  in order to be compared to the typical mass terms for neutral bosons, therefore using Eqn. 1.29

$$\begin{aligned} \frac{1}{8} v^2 [g^2 (W_\mu^3)^2 - 2gg' W_\mu^3 B^\mu + g'^2 B_\mu^2] &= \frac{1}{8} v^2 [g W_\mu^3 - g' B_\mu]^2 + 0[g' W_\mu^3 + g B_\mu]^2 \quad (1.46) \\ &= \frac{1}{8} v^2 [\sqrt{g^2 + g'^2} Z_\mu]^2 + 0[\sqrt{g^2 + g'^2} A_\mu]^2 \end{aligned}$$

825 and then

$$M_Z = \frac{1}{2} v \sqrt{g^2 + g'^2}, \quad M_A = 0 \quad (1.47)$$

826 **1.3.4 Masses of the fermions**

827 The lepton mass terms can be generated by introducing a gauge invariant Lagrangian  
 828 term describing the Yukawa coupling between the lepton field and the Higgs field

$$\mathcal{L}_{Yl} = -G_l \left[ (\bar{\nu}_l, \bar{l})_L \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} l_R + \bar{l}_R (\phi^-, \bar{\phi}^0) \begin{pmatrix} \nu_l \\ l \end{pmatrix} \right], \quad l = e, \mu, \tau. \quad (1.48)$$

829 After the SSB and replacing the usual field expansion about the ground state  
 830 (Eqn.1.41) into  $\mathcal{L}_{Yl}$ , the mass term arises

$$\mathcal{L}_{Yl} = -m_l (\bar{l}_L l_R + \bar{l}_R l_L) - \frac{m_l}{v} (\bar{l}_L l_R + \bar{l}_R l_L) H = -m_l \bar{l} l \left( 1 + \frac{H}{v} \right) \quad (1.49)$$

831

$$m_l = \frac{G_l}{\sqrt{2}} v \quad (1.50)$$

832 where the additional term represents the lepton-Higgs interaction. The quark masses  
 833 are generated in a similar way as lepton masses but for the upper member of the  
 834 quark doublet a different Higgs doublet is needed:

$$\phi_c = -i\sigma_2 \phi^* = \begin{pmatrix} -\bar{\phi}^0 \\ \phi^- \end{pmatrix}. \quad (1.51)$$

835 Additionally, given that the quark isospin doublets are not constructed in terms  
 836 of the mass eigenstates but in terms of the flavor eigenstates, as shown in Table 1.5,  
 837 the coupling parameters will be related to the CKM matrix elements; thus, the quark  
 838 Lagrangian is given by:

$$\mathcal{L}_{Yq} = -G_d^{i,j} (\bar{u}_i, \bar{d}'_i)_L \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} d_{jR} - G_u^{i,j} (\bar{u}_i, \bar{d}'_i)_L \begin{pmatrix} -\bar{\phi}^0 \\ \phi^- \end{pmatrix} u_{jR} + h.c. \quad (1.52)$$

839 with  $i, j = 1, 2, 3$ . After SSB and expansion about the ground state, the diagonal form

840 of  $\mathcal{L}_{Yq}$  is:

$$\mathcal{L}_{Yq} = -m_d^i \bar{d}_i d_i \left(1 + \frac{H}{v}\right) - m_u^i \bar{u}_i u_i \left(1 + \frac{H}{v}\right) \quad (1.53)$$

841 Fermion masses depend on arbitrary couplings  $G_l$  and  $G_{u,d}$  and are not predicted  
842 by the theory.

### 843 1.3.5 The Higgs field

844 After the characterization of the fermions and gauge bosons as well as their interac-  
845 tions, it is necessary to characterize the Higgs field itself. The Lagrangian  $\mathcal{L}_S$  in Eqn.  
846 1.37 written in terms of the gauge bosons is given by

$$\mathcal{L}_S = \frac{1}{4} \lambda v^4 + \mathcal{L}_H + \mathcal{L}_{HV} \quad (1.54)$$

847

$$\mathcal{L}_H = \frac{1}{2} \partial_\mu H \partial^\mu H - \frac{1}{2} m_H^2 H^2 - \frac{1}{2v} m_H^2 H^3 - \frac{1}{8v^2} m_H^2 H^4 \quad (1.55)$$

848

$$\mathcal{L}_{HV} = m_H^2 W_\mu^+ W^{\mu-} \left(1 + \frac{2}{v} H + \frac{2}{v^2} H^2\right) + \frac{1}{2} m_Z^2 Z_\mu Z^\mu \left(1 + \frac{2}{v} H + \frac{2}{v^2} H^2\right) \quad (1.56)$$

849 The mass of the Higgs boson is deduced as usual from the mass term in the Lagrangian  
850 resulting in:

$$m_H = \sqrt{-2\mu^2} = \sqrt{2\lambda}v \quad (1.57)$$

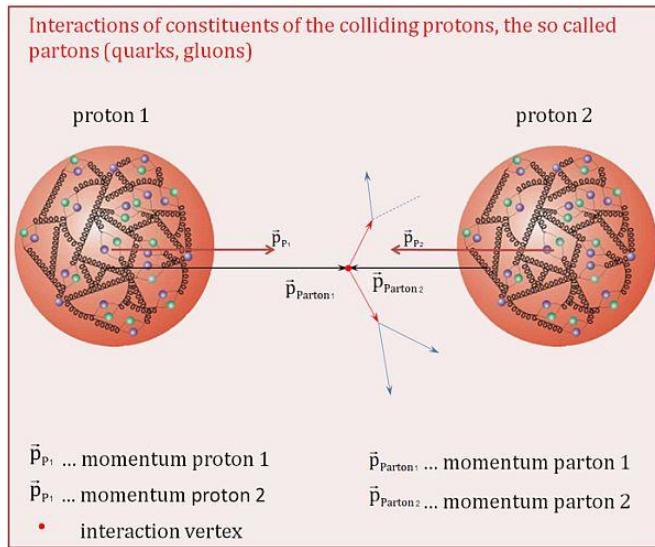
851 however, it is not predicted by the theory either. The experimental measurement of  
852 the Higgs boson mass have been performed by the *Compact Muon Solenoid (CMS)*  
853 experiment and the *A Toroidal LHC Appartus (ATLAS)* experiments at the *Large  
854 Hadron Collider (LHC)*, [36–38], and is presented in Table 1.8.

Property	Value
Electric charge	0
Color charge	0
Spin	0
Weak isospin	-1/2
Weak hypercharge	1
Parity	1
Mass (GeV/c <sup>2</sup> )	125.09±0.21 (stat.)±0.11 (syst.)

**Table 1.8:** Higgs boson properties. Higgs mass is not predicted by the theory and the value here corresponds to the experimental measurement.

### 1.3.6 Production of Higgs bosons at LHC

857 At the LHC, Higgs bosons are produced as a result of the collision of two counter-  
858 rotating protons beams. A detailed description of the LHC machine will be presented  
in chapter 2.



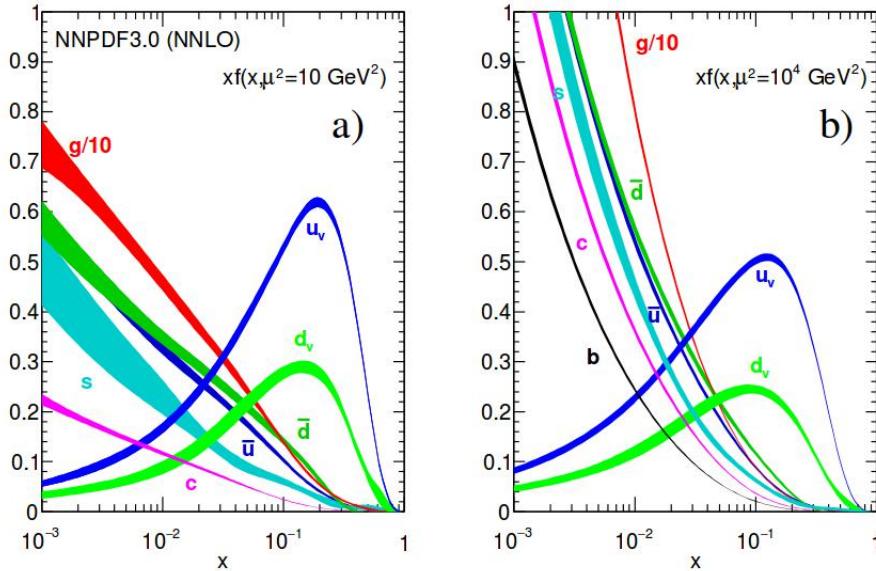
**Figure 1.10:** Proton-proton collision. Protons are composed of 3 valence quarks, a sea of quarks and gluons; therefore in a proton-proton collision, quarks and gluons are those who collide. [39].

859

860 Protons are composed of quarks and these quarks are bound by gluons; however,  
861 what is commonly called the quark content of the proton makes reference to the  
862 valence quarks. In fact, a proton is not just a rigid entity with three balls in it all  
863 tied up with springs, but the gluons exchanged by the valence quarks tend to split

864 spontaneously into quark-antiquark pairs or more gluons, creating *sea of quarks and*  
 865 *gluons* as represented in Figure 1.10.

866 In a proton-proton ( $pp$ ) collision, the proton's constituents, quarks and gluons, are  
 867 those that collide. The  $pp$  cross section depends on the momentum of the colliding  
 868 particles, reason for which it is needed to know how the momentum is distributed  
 869 inside the proton. Quarks and gluons are known as partons, hence, the functions  
 870 that describe how the proton momentum is distributed among partons inside it are  
 871 called *parton distribution functions (PDFs)*; PDFs are determined from experimental  
 872 data obtained in experiments where the internal structure of hadrons is tested, and  
 873 depend on the momentum transfer  $Q$  and the fraction of momentum  $x$  carried by an  
 874 specific parton. Figure 1.11 shows the proton PDFs ( $xf(x, Q^2)$ ) for two values of  $Q$ .

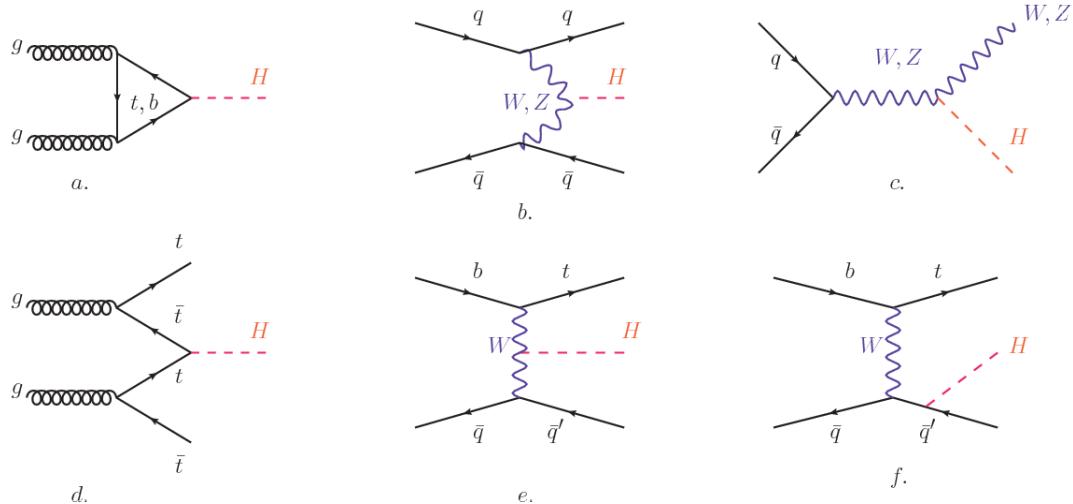


**Figure 1.11:** Proton PDFs for two values of  $Q^2$ : left.  $\mu^2 = Q^2 = 10 \text{ GeV}^2$ , right.  $\mu^2 = Q^2 = 10^4 \text{ GeV}^2$ .  $u_v$  and  $d_v$  correspond to the  $u$  and  $d$  valence quarks,  $s, c, b, \bar{u}, \bar{d}$  correspond to sea quarks, and  $g$  corresponds to gluons. Note that gluons carry a high fraction of the proton's momentum. [9]

875 In physics, a common approach to study complex systems consists of starting  
 876 with a simpler version of them, for which a well known description is available, and

adding an additional *perturbation* which represents a small deviation from the known behavior. If the perturbation is small enough, the physical quantities associated with the perturbed system are expressed as a series of corrections to those of the simpler system. The perturbation series corresponds to an expansion in power series of a small parameter, therefore, the more terms are considered in the series (the higher order in the perturbation series), the more precise is the description of the complex system. If the perturbation does not get progressively smaller, the strategy cannot be applied and new methods have to be employed.

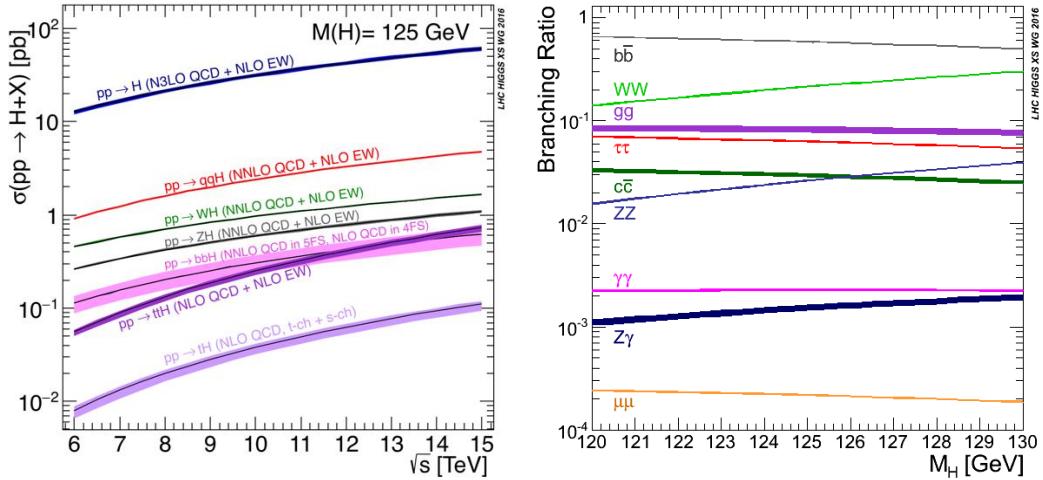
High energy systems, like the Higgs production at LHC explored in this thesis, usually can be treated perturbatively with the expansion made in terms of the coupling constants. The overview presented here will be oriented specifically to the Higgs boson production mechanisms in  $pp$  collisions at LHC.



**Figure 1.12:** Main Higgs boson production mechanism Feynman diagrams. a. gluon-gluon fusion, b. vector boson fusion (VBF), c. Higgs-strahlung, d. Associated production with a top or bottom quark pair, e-f. associated production with a single top quark.

Figure 1.12 shows the Feynman diagrams for the leading order (first order) Higgs production processes at LHC; note that in these diagrams the incoming particles are not the protons themselves but the partons from the protons that actually participate

in the interaction, hence, theorists typically calculate the cross section for the parton interaction, and then convolute that cross section with the information from the PDFs to get a production cross section that is actually measured in experiments. The cross section for Higgs production as a function of the center of mass-energy ( $\sqrt{s}$ ) for  $pp$  collisions is showed in Figure 1.13 left. The tags NLO (next to leading order), NNLO (next to next to leading order) and N3LO (next to next to next to leading order) make reference to the order at which the perturbation series have been considered while the tags QCD and EW correspond to the strong and electroweak coupling constants respectively.



**Figure 1.13:** Higgs boson production cross sections (left) and decay branching ratios (right) for the main mechanisms. The VBF is indicated as  $qqH$  [40].

The main production mechanism is the gluon fusion (Figure 1.12a and  $pp \rightarrow H$  in Figure 1.13) given that gluons carry the highest fraction of momentum of the protons in  $pp$  colliders (as shown in Figure ??). Since the Higgs boson does not couple to gluons, the mechanism proceeds through the exchange of a virtual top-quark loop. Note that in this process the Higgs boson is produced alone, turning out to be problematic for some Higgs decays, because such absence of anything produced in

907 association with the Higgs represent a trouble for triggering, however, this mechanism  
 908 is experimentally clean when combined with the two-photon or the four-lepton decay  
 909 channels (see Section 1.3.7).

910 Vector boson fusion (Figure 1.12b and  $pp \rightarrow qqH$  in Figure 1.13) has the second  
 911 largest production cross section. The scattering of two fermions is mediated by a weak  
 912 gauge boson which later emits a Higgs boson. In the final state, the two fermions tend  
 913 to be located in the central region of the detector; this kind of features are generally  
 914 used as a signature when analyzing the datasets provided by the experiments<sup>7</sup>.

915 In the Higgs-strahlung mechanism (Figure 1.12c and  $pp \rightarrow WH, pp \rightarrow ZH$  in  
 916 Figure 1.13) two fermions annihilate to form a weak gauge boson. If the initial  
 917 fermions have enough energy, the emergent boson might emit a Higgs boson.

918 The associated production with a top or bottom quark pair and the associated  
 919 production with a single top quark (Figure 1.12d-f and  $pp \rightarrow bbH, pp \rightarrow t\bar{t}H, pp \rightarrow tH$   
 920 in Figure 1.13) have a smaller cross section than the main three mechanisms above,  
 921 but they provide a good opportunity to test the Higgs-top coupling. The analysis  
 922 reported in this thesis is developed using these production mechanisms. A detailed  
 923 description of the  $tH$  mechanism will be given in Section 1.5.

### 924 1.3.7 Higgs boson decay channels

925 When a particle can decay through several modes, also known as channels, the prob-  
 926 ability of decaying through a given channel is quantified by the *branching ratio (BR)*  
 927 of the decay channel; thus, the BR is defined as the ratio of number of decays go-  
 928 ing through that given channel to the total number of decays. In regard to the  
 929 Higgs boson decay, the BR can be predicted with accuracy once the Higgs mass is  
 930 known [41, 42]. In Figure 1.13 right, a plot of the BR as a function of the Higgs mass

---

<sup>7</sup> More details about how to identify events of interest in this analysis will be given in chapter 6.

931 is presented; the largest predicted BR corresponds to the  $b\bar{b}$  pair decay channel (see  
 932 Table 1.9) given that it is the heaviest particle pair whose on-shell<sup>8</sup> production is  
 933 kinematically allowed in the decay.

Decay channel	Branching ratio	Rel. uncertainty
$H \rightarrow b\bar{b}$	$5.84 \times 10^{-1}$	+3.2% – 3.3%
$H \rightarrow W^+W^-$	$2.14 \times 10^{-1}$	+4.3% – 4.2%
$H \rightarrow \tau^+\tau^-$	$6.27 \times 10^{-2}$	+5.7% – 5.7%
$H \rightarrow ZZ$	$2.62 \times 10^{-2}$	+4.3% – 4.1%
$H \rightarrow \gamma\gamma$	$2.27 \times 10^{-3}$	+5.0% – 4.9%
$H \rightarrow Z\gamma$	$1.53 \times 10^{-3}$	+9.0% – 8.9%
$H \rightarrow \mu^+\mu^-$	$2.18 \times 10^{-4}$	+6.0% – 5.9%

**Table 1.9:** Predicted branching ratios and the relative uncertainty for some decay channels of a SM Higgs boson with  $m_H = 125\text{GeV}/c^2$  [9]; the uncertainties are driven by theoretical uncertainties for the different Higgs boson partial widths and by parametric uncertainties associated to the strong coupling and the masses of the quarks which are the input parameters. Further details on these calculations can be found in Reference [43]

934

935 Decays to other lepton and quark pairs, like electron, strange, up, and down  
 936 quark pairs not listed in the table, are also possible but their likelihood is too small  
 937 to measure since they are very lightweight, hence, their interaction with the Higgs  
 938 boson is very weak. On other hand, the decay to top quark pairs is heavily suppressed  
 939 due to the top quark mass ( $\approx 173\text{ GeV}/c^2$ ).

940 Decays to gluons proceed indirectly through a virtual top quark loop while the  
 941 decays to photons proceed through a virtual W boson loop, therefore, their branching  
 942 ratio is smaller compared to direct interaction decays. Same is true for the decay to  
 943 a photon and a Z boson.

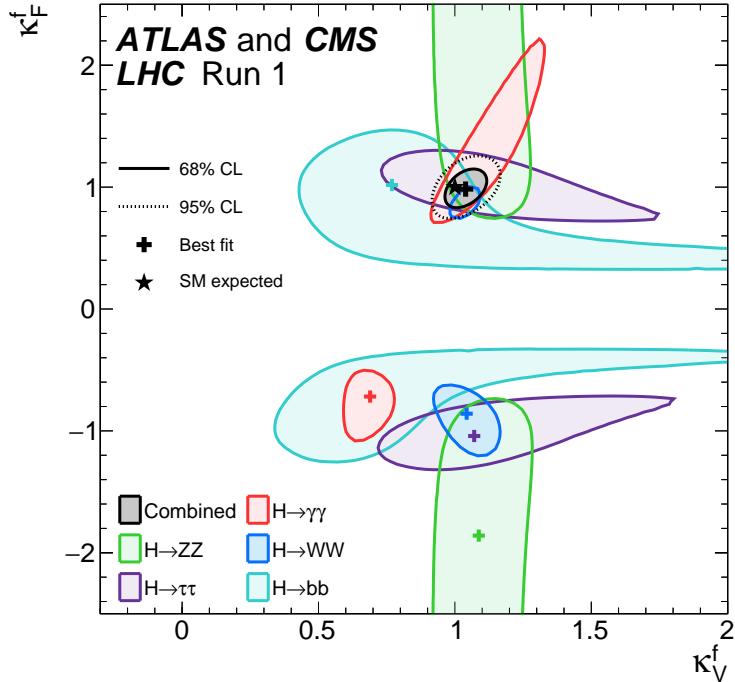
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<sup>8</sup> In general, on-shell or real particles are those which satisfy the energy-momentum relation ( $E^2 - |\vec{p}|^2 c^2 = m^2 c^4$ ); off-shell or virtual particles does not satisfy it which is possible under the uncertainty principle of quantum mechanics. Usually, virtual particles correspond to internal propagators in Feynman diagrams.

944 In the case of decays to pairs of W and Z bosons, the decay proceed with one of  
 945 the bosons being on-shell and the other being off-shell. The likelihood of the process  
 946 diminish depending on how far off-shell are the virtual particles involved, hence, the  
 947 branching ratio for W boson pairs is bigger than for Z boson pairs since Z boson mass  
 948 is bigger than W boson mass.

949 Note that the decay to a pair of virtual top quarks is possible, but the probability  
 950 is way too small.

951 **1.4 Experimental status of the anomalous  
 952 Higgs-fermion coupling**



**Figure 1.14:** Combination of the ATLAS and CMS fits for coupling modifiers  $\kappa_t - \kappa_V$ ; also shown the individual decay channels combination and their global combination. No assumptions have been made on the sign of the coupling modifiers [44].

953       ATLAS and CMS have performed analyses of the anomalous Higgs-fermion cou-  
 954 pling by making likelihood scans for the two coupling modifiers,  $\kappa_f$  and  $\kappa_V$ , under  
 955 the assumption that  $\kappa_Z = \kappa_W \equiv \kappa_V$  and  $\kappa_t = \kappa_\tau = \kappa_b \equiv \kappa_f$ . Figure 1.14 shows the  
 956 result of the combination of ATLAS and CMS fits; also the individual decay channels  
 957 combination and the global combination results are shown. Note that from this plot  
 958 there is limited information on the sign of the coupling since the only information  
 959 available about the sign of the coupling comes from decays rather than production.

960       While all the channels are compatible for positive values of the modifiers, for  
 961 negative values of  $\kappa_f$  there is no compatibility. The best fit for individual channels  
 962 is compatible with negative values of  $\kappa_f$  except for the  $H \rightarrow bb$  channel. The best  
 963 fit for the combination yields  $\kappa_f \geq 0$ , in contrast to the yields from the individual  
 964 channels; the reason of this yield resides in the  $H \rightarrow \gamma\gamma$  coupling.  $H \rightarrow \gamma\gamma$  decay  
 965 proceeds through a loop of either top quarks or W bosons, hence, this channel is  
 966 sensitive to  $\kappa_t$  thanks to the interference of these two amplitude contributions; under  
 967 the assumption that no beyond SM particles take part in the loops, a flipped sign  
 968 of  $\kappa_t$  will increase the  $H \rightarrow \gamma\gamma$  branching fraction by a factor of  $\sim 2.4$  which is not  
 969 supported by measurements; thus, this large asymmetry between the positive and  
 970 negative coupling ratios in the  $H \rightarrow \gamma\gamma$  channel drives the yield of the global fit and  
 971 would mean that the anomalous H-t coupling is excluded as stated in Reference [44],  
 972 but there is a caveat, this exclusion holds only if no new particles contribute to the  
 973 loop in the main diagram for that decay.

974       Although the  $H \rightarrow bb$  channel is expected to be the most sensitive channel and  
 975 its best fit value of  $\kappa_t$  is positive, and then the global fit yield is still supported,  
 976 the contributions from all the other decay channels, small compared to the  $H \rightarrow bb$ ,  
 977 indicate that the anomalous H-t coupling cannot be excluded completely, motivating  
 978 to look at  $tH$  processes which can help with both, the limited information on the sign

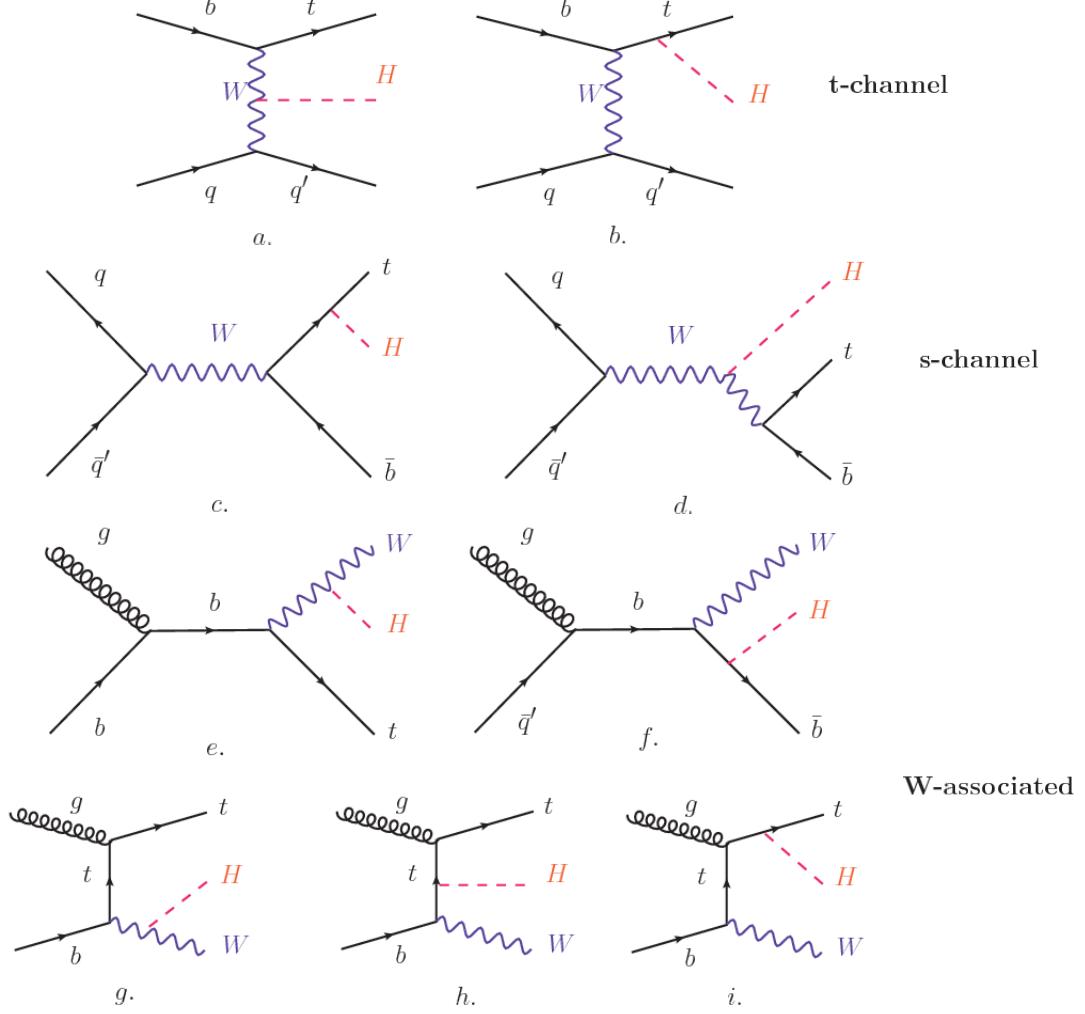
979 of the H-t coupling and the access to information from the Higgs boson production  
 980 rather than from its decays.

981 It will be shown in Section 1.5 that the same interference effect enhance the  $tH$   
 982 production rate and could reveal evidence of direct production of heavy new particles  
 983 as predicted in composite and little Higgs models [45], or new physics related to  
 984 Higgs boson mediated flavor changing neutral currents [46] as well as probes the  
 985 CP-violating phase of the H-t coupling [47, 48].

## 986 1.5 Associated production of a Higgs boson and a 987 single top quark

988 The production of Higgs boson in association with a top quark has been extensively  
 989 studied [47, 49–52]. While measurements of the main Higgs production mechanisms  
 990 rates are sensitive to the strength of the Higgs coupling to W boson or top quark,  
 991 they are not sensitive to the relative sign between the two couplings. In this thesis,  
 992 the Higgs boson production mechanism explored is the associated production with a  
 993 single top quark ( $tH$ ) which offers sensitivity to the relative sign of the Higgs couplings  
 994 to W boson and to top quark. The description given here is based on Reference [51]

A process where two incoming particles interact and produce a final state with two particles can proceed in three called channels (see, for instance, Figure 1.15 omitting the red line). The t-channel represents processes where an intermediate particle is emitted by one of the incoming particles and absorbed by the other. The s-channel represents processes where the two incoming particles merge into an intermediate particle which eventually will split into the particles in the final state. The third channel, u-channel, is similar to the t-channel but the two outgoing particles interchange their



**Figure 1.15:** Associated Higgs boson production with a top quark mechanism Feynman diagrams. a.,b. t-channel ( $tHq$ ), c.,d. s-channel ( $tHb$ ), e-i. W-associated.

roles. These three channels are connected to the so-called Mandelstam variables

$$s = (p_1 + p_2)^2 = (p'_1 + p'_2)^2 \rightarrow \text{square of the center mass-energy.} \quad (1.58)$$

$$t = (p_1 - p'_1)^2 = (p'_2 - p_2)^2 \rightarrow \text{square of the four-momentum transfer.} \quad (1.59)$$

$$u = (p_1 - p'_2)^2 = (p'_1 - p_2)^2 \rightarrow \text{square of the crossed four-momentum transfer.} \quad (1.60)$$

$$s + t + u = m_1^2 + m_2^2 + m'_1^2 + m'_2^2 \quad (1.61)$$

which relate the momentum, energy and the angles of the incoming and outgoing particles in an scattering process of two particles to two particles. The importance of the Mandelstam variables reside in that they form a minimum set of variables needed to describe the kinematics of this scattering process; they are Lorentz invariant which makes them very useful when doing calculations.

The  $tH$  production, where Higgs boson can be radiated either from the top quark or from the W boson, is represented by the leading order Feynman diagrams in Figure 1.15. The cross section for the  $tH$  process is calculated, as usual, summing over the contributions from the different Feynman diagrams; therefore it depends on the interference between the contributions. In the SM, the interference for t-channel ( $tHq$  process) and W-associated ( $tHW$  process) production is destructive [49] resulting in the small cross sections presented in Table 1.10.

tH production channel	Cross section (fb)
t-channel ( $pp \rightarrow tHq$ )	$70.79^{+2.99}_{-4.80}$
W-associated ( $pp \rightarrow tHW$ )	$15.61^{+0.83}_{-1.04}$
s-channel( $pp \rightarrow tHb$ )	$2.87^{+0.09}_{-0.08}$

**Table 1.10:** Predicted SM cross sections for  $tH$  production at  $\sqrt{s} = 13$  TeV [53, 54].

The s-channel contribution can be neglected. It will be shown that a deviation from the SM destructive interference would result in an enhancement of the  $tH$  cross section compared to that in SM, which could be used to get information about the sign of the Higgs-top coupling [51, 52]. In order to describe  $tH$  production processes, Feynman diagram 1.15b will be considered; there, the W boson is radiated by a quark in the proton and eventually it will interact with the b quark. In the high energy regime, the effective W approximation [55] is used to describe the process as the

1015 emission of an approximately on-shell W and its hard scattering with the b quark;  
 1016 i.e.  $Wb \rightarrow th$ . The scattering amplitude for the process is given by

$$\mathcal{A} = \frac{g}{\sqrt{2}} \left[ (\kappa_t - \kappa_V) \frac{m_t \sqrt{s}}{m_W v} A \left( \frac{t}{s}, \varphi; \xi_t, \xi_b \right) + \left( \kappa_V \frac{2m_W s}{v t} + (2\kappa_t - \kappa_V) \frac{m_t^2}{m_W v} \right) B \left( \frac{t}{s}, \varphi; \xi_t, \xi_b \right) \right], \quad (1.62)$$

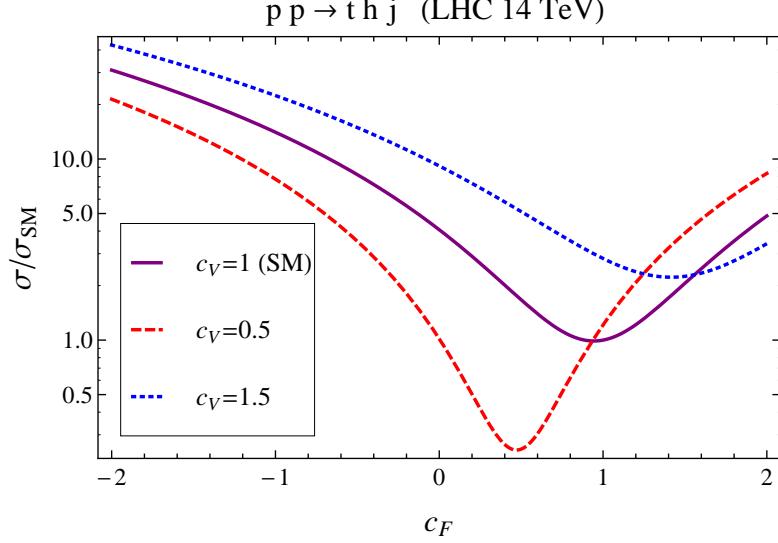
1017 where  $\kappa_V \equiv g_{HVV}/g_{HVV}^{SM}$  and  $\kappa_t \equiv g_{Ht}/g_{Ht}^{SM} = y_t/y_t^{SM}$  are scaling factors that quantify  
 1018 possible deviations of the couplings from the SM values, Higgs-Vector boson (H-  
 1019 W) and Higgs-top (H-t) respectively, from the SM couplings;  $s = (p_W + p_b)^2$ ,  $t =$   
 1020  $(p_W - p_H)^2$ ,  $\varphi$  is the Higgs azimuthal angle around the  $z$  axis taken parallel to the  
 1021 direction of motion of the incoming W; A and B are functions describing the weak  
 1022 interaction in terms of the chiral states  $(\xi_t, \xi_b)$  of the quarks  $b$  and  $t$ . Terms that  
 1023 vanish in the high energy limit have been neglected as well as the Higgs and  $b$  quark  
 1024 masses<sup>9</sup>.

1025 The scattering amplitude grows with energy like  $\sqrt{s}$  for  $\kappa_V \neq \kappa_t$ , in contrast to  
 1026 the SM ( $\kappa_t = \kappa_V = 1$ ), where the first term in 1.62 cancels out and the amplitude  
 1027 is constant for large  $s$ ; therefore, a deviation from the SM predictions represents an  
 1028 enhancement in the  $tHq$  cross section. In particular, for a SM H-W coupling and a  
 1029 H-t coupling of inverted sign with respect to the SM ( $\kappa_V = -\kappa_t = 1$ ) the  $tHq$  cross  
 1030 section is enhanced by a factor greater 10 as seen in the Figure 1.16 taken from  
 1031 Reference [51]; Reference [56] has reported similar enhancement results.

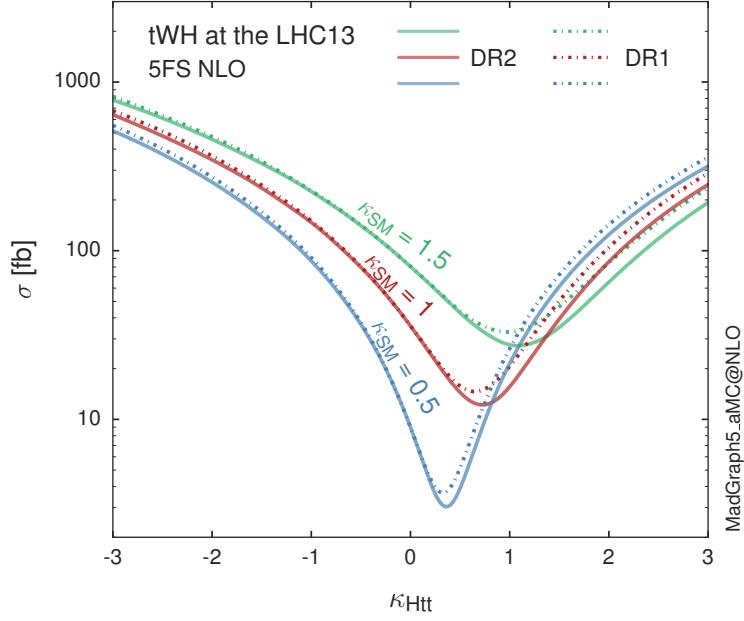
1032 A similar analysis is valid for the W-associated channel but, in that case, the in-  
 1033 terference is more complicated since there are more than two contributions and an ad-  
 1034 ditional interference with the production of Higgs boson and a top pair process( $t\bar{t}H$ ).  
 1035 The calculations are made using the so-called Diagram Removal (DR) technique where

---

<sup>9</sup> A detailed explanation of the structure and approximations used to derive  $\mathcal{A}$  can be found in Reference [51]



**Figure 1.16:** Cross section for  $tHq$  process as a function of  $\kappa_t$ , normalized to the SM, for three values of  $\kappa_V$ . In the plot  $c_f$  refers to the Higgs-fermion coupling which is dominated by the H-t coupling and represented here by  $\kappa_t$ . Solid, dashed and dotted lines correspond to  $c_V \rightarrow \kappa_V = 1, 0.5, 1.5$  respectively. Note that for the SM ( $\kappa_V = \kappa_t = 1$ ), the destructive effect of the interference is maximal.



**Figure 1.17:** Cross section for  $tHW$  process as a function of  $\kappa_{Htt}$ , for three values of  $\kappa_{SM}$  at  $\sqrt{s} = 13$  TeV.  $\kappa_{Htt}^2 = \sigma_{Htt}/\sigma_{Htt}^{SM}$  is a simple re-scaling of the SM Higgs interactions.

interfering diagrams are removed (or added) from the calculations in order to evaluate the impact of the removed contributions. DR1 was defined to neglect  $t\bar{t}H$  interference while DR2 was defined to take  $t\bar{t}H$  interference into account [48]. As shown in Figure 1.17, the  $tHW$  cross section is enhanced from about 15 fb (SM:  $\kappa_{Htt} = 1$ ) to about 150 fb ( $\kappa_{Htt} = -1$ ). Differences between curves for DR1 and DR2 help to gauge the impact of the interference with  $t\bar{t}H$ . Results of the calculations of the  $tHq$  and  $tHW$  cross sections at  $\sqrt{s} = 13$  TeV can be found in Reference [57] and a summary of the results is presented in Table 1.11.

	$\sqrt{s}$ TeV	$\kappa_t = 1$	$\kappa_t = -1$
$\sigma^{LO}(tHq)(fb)$ [51]	8	$\approx 17.4$	$\approx 252.7$
	14	$\approx 80.4$	$\approx 1042$
$\sigma^{NLO}(tHq)(fb)$ [51]	8	$18.28^{+0.42}_{-0.38}$	$233.8^{+4.6}_{-0.0}$
	14	$88.2^{+1.7}_{-0.0}$	$982.8^{+28}_{-0.0}$
$\sigma^{LO}(tHq)(fb)$ [56]	14	$\approx 71.8$	$\approx 893$
$\sigma^{LO}(tHW)(fb)$ [56]	14	$\approx 16.0$	$\approx 139$
$\sigma^{NLO}(tHq)(fb)$ [57]	8	$18.69^{+8.62\%}_{-17.13\%}$	-
	13	$74.25^{+7.48\%}_{-15.35\%}$	$848^{+7.37\%}_{-13.70\%}$
	14	$90.10^{+7.34\%}_{-15.13\%}$	$1011^{+7.24\%}_{-13.39\%}$
$\sigma^{LO}(tHW)(fb)$ [48]	13	$15.77^{+15.91\%}_{-15.76\%}$	-
$\sigma^{NLO}DR1(tHW)(fb)$ [48]	13	$21.72^{+6.52\%}_{-5.24\%}$	$\approx 150$
$\sigma^{NLO}DR2(tHW)(fb)$ [48]	13	$16.28^{+7.34\%}_{-15.13\%}$	$\approx 150$

**Table 1.11:** Predicted enhancement of the  $tHq$  and  $tHW$  cross sections at LHC for  $\kappa_V = 1$  and  $\kappa_t = \pm 1$  at LO and NLO; the cross section enhancement of more than a factor of 10 is due to the flipping in the sign of the H-t coupling with respect to the SM one.

1044

## 1045 1.6 CP-mixing in $tH$ processes

1046 In addition to the sensitivity to sign of the H-t coupling, the  $tHq$  and  $tHW$  processes  
 1047 have been proposed as a tool to investigate the possibility of a H-t coupling that does

1048 not conserve CP [47, 48, 58].

1049 In this thesis, the sensitivity of  $tH$  processes to CP-mixing is also studied on the  
 1050 basis of References [47, 48] using the effective field theory framework where a generic  
 1051 particle ( $X_0$ ) of spin-0 and a general CP violating interaction with the top quark  
 1052 ( $Htt$  coupling), can couple to scalar and pseudo-scalar fermionic densities. The H-W  
 1053 interaction is assumed to be SM-like. The Lagrangian modeling the H-t interaction  
 1054 is given by

$$\mathcal{L}_0^t = -\bar{\psi}_t (c_\alpha \kappa_{Htt} g_{Htt} + i s_\alpha \kappa_{Att} g_{Att} \gamma_5) \psi_t X_0, \quad (1.63)$$

1055 where  $\alpha$  is the CP-mixing phase,  $c_\alpha \equiv \cos \alpha$  and  $s_\alpha \equiv \sin \alpha$ ,  $\kappa_{Htt}$  and  $\kappa_{Att}$  are real  
 1056 dimensionless re-scaling parameters<sup>10</sup> used to parametrize the magnitude of the CP-  
 1057 violating and CP-conserving parts of the amplitude. The model defines  $g_{Htt} =$   
 1058  $g_{Att} = m_t/v = y_t/\sqrt{2}$  with  $v \sim 246$  GeV the Higgs vacuum expectation value. In  
 1059 this parametrization, three special cases can be recovered

1060 • CP-even coupling  $\rightarrow \alpha = 0^\circ$

1061 • CP-odd coupling  $\rightarrow \alpha = 90^\circ$

1062 • SM coupling  $\rightarrow \alpha = 0^\circ$  and  $\kappa_{Htt} = 1$

1063 The loop induced  $X_0$  coupling to gluons can also be described in terms of the  
 1064 parametrization above, according to

$$\mathcal{L}_0^g = -\frac{1}{4} \left( c_\alpha \kappa_{Hgg} g_{Hgg} G_{\mu\nu}^a G^{a,\mu\nu} + s_\alpha \kappa_{Agg} g_{Agg} G_{\mu\nu}^a \tilde{G}^{a,\mu\nu} \right) X_0. \quad (1.64)$$

1065 where  $g_{Hgg} = -\alpha_s/3\pi v$  and  $g_{Agg} = \alpha_s/2\pi v$  and  $G_{\mu\nu}$  is the gluon field strength tensors.

1066 Under the assumption that the top quark dominates the gluon-fusion process at LHC

---

<sup>10</sup> analog to  $\kappa_t$  and  $\kappa_V$

1067 energies,  $\kappa_{Hgg} \rightarrow \kappa_{Htt}$  and  $\kappa_{Agg} \rightarrow \kappa_{Att}$ , so that the ratio between the gluon-gluon  
 1068 fusion cross section for  $X_0$  and for the SM Higgs prediction can be written as

$$\frac{\sigma_{NLO}^{gg \rightarrow X_0}}{\sigma_{NLO,SM}^{gg \rightarrow H}} = c_\alpha^2 \kappa_{Htt}^2 + s_\alpha^2 \left( \kappa_{Att} \frac{g_{Agg}}{g_{Hgg}} \right)^2. \quad (1.65)$$

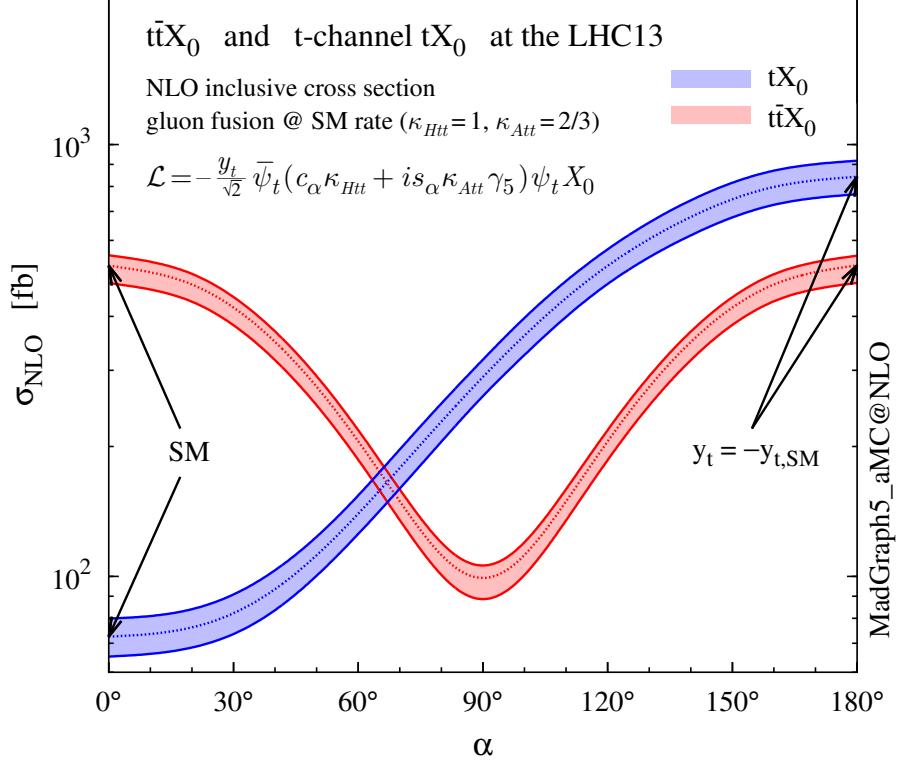
1069 If the re-scaling parameters are set to

$$\kappa_{Htt} = 1, \quad \kappa_{Att} = \left| \frac{g_{Hgg}}{g_{Agg}} \right| = \frac{2}{3}. \quad (1.66)$$

1070 the gluon-fusion SM cross section is reproduced for every value of the CP-mixing  
 1071 angle  $\alpha$ ; therefore, by imposing that condition to the Lagrangian density 1.63, the  
 1072 CP-mixing angle is not constrained by current data. Figure 1.18 shows the NLO cross  
 1073 sections for t-channel  $tX_0$ (blue) and  $t\bar{t}X_0$  (red) associated production processes as a  
 1074 function of the CP-mixing angle  $\alpha$ .  $X_0$  is a generic spin-0 particle with top quark  
 1075 CP-violating coupling. Re-scaling factors  $\kappa_{Htt}$  and  $\kappa_{Att}$  have been set to reproduce  
 1076 the SM gluon-fusion cross sections.

1077 It is interesting to notice that the  $tX_0$  cross section is enhanced, by a factor of  
 1078 about 10, when a continuous rotation in the scalar-pseudoscalar plane is applied; this  
 1079 enhancement is similar to the enhancement produced when the H-t coupling is flipped  
 1080 in sign with respect to the SM ( $y_t = -y_{t,SM}$  in the plot), as showed in Section 1.5. In  
 1081 contrast, the degeneracy in the  $t\bar{t}X_0$  cross section is still present given that it depends  
 1082 quadratically on the H-t coupling, but more interesting is to notice that  $t\bar{t}X_0$  cross  
 1083 section is exceeded by  $tX_0$  cross section after  $\alpha \sim 60^\circ$ .

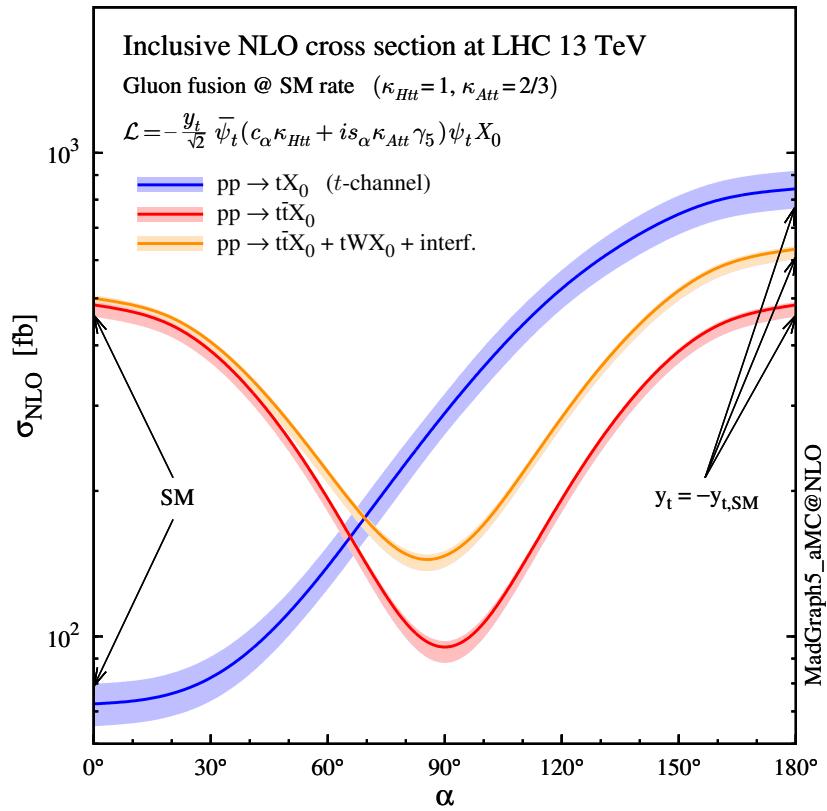
1084 A similar parametrization can be used to investigate the  $tHW$  process sensitivity  
 1085 to CP-violating H-t coupling. As said in 1.5, the interference in the W-associated  
 1086 channel is more complicated because there are more than two contributions and also  
 1087 there is interference with the  $t\bar{t}H$  production process.



**Figure 1.18:** NLO cross sections for t-channel  $tX_0$ (blue) and  $t\bar{t}X_0$  (red) associated production processes as a function of the CP-mixing angle  $\alpha$ .  $X_0$  is a generic spin-0 particle with top quark CP-violating coupling [47].

1088     Figure 1.19 shows the NLO cross sections for t-channel  $tX_0$ (blue),  $t\bar{t}X_0$  (red)  
 1089     associated production and for the combined  $tWX_0+t\bar{t}X_0+interference$  (orange) as  
 1090     a function of the CP-mixing angle. It is clear that the effect of the interference in the  
 1091     combined case is the lifting of the degeneracy present in the  $t\bar{t}X_0$  production. The  
 1092     constructive interference enhances the cross section from about 500 fb at SM ( $\alpha = 0$ )  
 1093     to about 600 fb ( $\alpha = 180^\circ \rightarrow y_t = -y_{t,SM}$ ).

1094     An analysis combining  $tHq$  and  $tHW$  processes will be made in this thesis taking  
 1095     advantage of the sensitivity improvement.



**Figure 1.19:** NLO cross sections for t-channel  $tX_0$  (blue),  $t\bar{t}X_0$  (red) associated production processes and combined  $tWX_0 + t\bar{t}X_0$  (including interference) production as a function of the CP-mixing angle  $\alpha$  [47].

<sub>1096</sub> **Chapter 2**

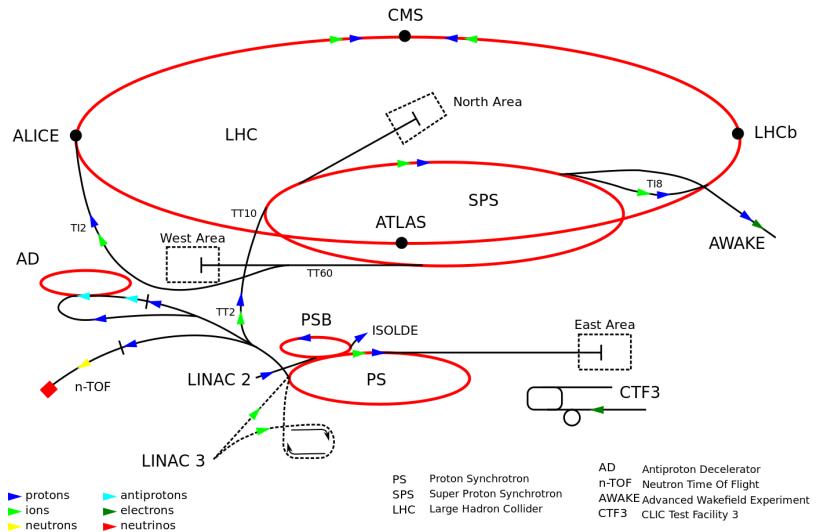
<sub>1097</sub> **The CMS experiment at the LHC**

<sub>1098</sub> **2.1 Introduction**

<sub>1099</sub> Located on the Swiss-French border, the European Council for Nuclear Research  
<sub>1100</sub> (CERN) is the largest scientific organization leading particle physics research. About  
<sub>1101</sub> 13000 people in a broad range of roles including users, students, scientists, engineers,  
<sub>1102</sub> among others, contribute to the data taking and analysis, with the goal of unveiling  
<sub>1103</sub> the secrets of nature and revealing the fundamental structure of the universe. CERN  
<sub>1104</sub> is also the home of the Large Hadron Collider (LHC), the largest particle accelerator  
<sub>1105</sub> around the world, where protons (or heavy ions) traveling close to the speed of light,  
<sub>1106</sub> are made to collide. These collisions open a window to investigate how particles (and  
<sub>1107</sub> their constituents if they are composite) interact with each other, providing clues  
<sub>1108</sub> about the laws of nature. This chapter presents an overview of the LHC structure  
<sub>1109</sub> and operation. A detailed description of the CMS detector is offered, given that the  
<sub>1110</sub> data used in this thesis have been taken with this detector.

## 2.2 The LHC

With 27 km of circumference, the LHC is currently the most powerful circular accelerator in the world. It is installed in the same tunnel where the Large Electron-Positron (LEP) collider was located, taking advantage of the existing infrastructure. The LHC is part of the CERN's accelerator complex composed of several successive acceleration stages before the particles are injected into the LHC ring where they reach their maximum energy (see Figure 2.1).



**Figure 2.1:** CERN accelerator complex. Blue arrows show the path followed by protons along the acceleration process [61].

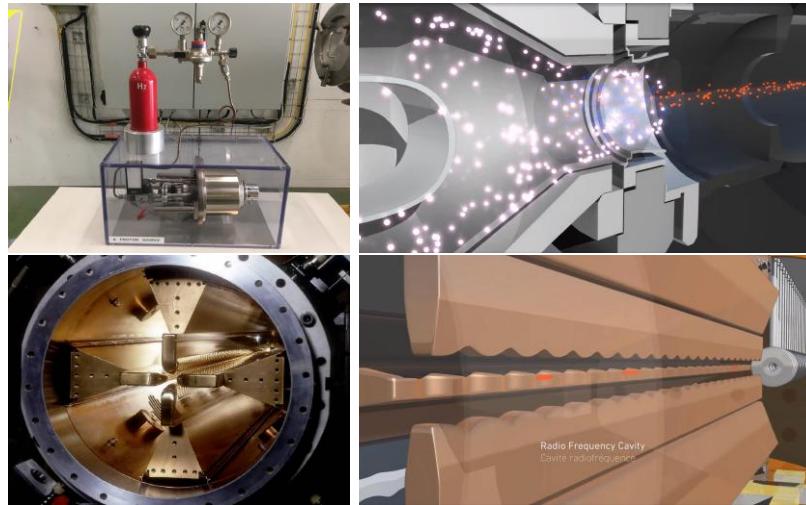
The LHC runs in three collision modes depending on the particles being accelerated

• Proton-Proton collisions ( $pp$ ) for multiple physics experiments.

• Lead-Lead collisions ( $Pb-Pb$ ) for heavy ion experiments.

• Proton-Lead collisions ( $p-Pb$ ) for quark-gluon plasma experiments.

In this thesis only  $pp$  collisions will be considered.

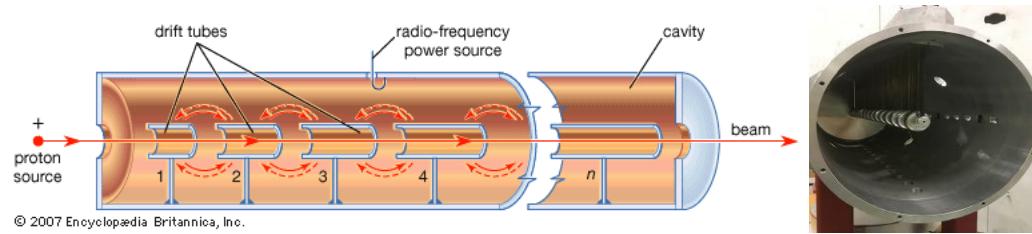


**Figure 2.2:** LHC protons source and the first acceleration stage. Top: the bottle contains hydrogen gas which is injected into the metal cylinder (white dots) to be broken down into electrons (blue dots) and protons (red dots); Bottom: the obtained protons are directed towards the radio frequency quadrupole which perform the first acceleration, focus the beam and create the bunches of protons. Left images are real pictures while right images are drawings [65, 66].

1124 Collection of protons starts with hydrogen atoms taken from a bottle, containing  
 1125 hydrogen gas, and injecting them in a metal cylinder; hydrogen atoms are broken  
 1126 down into electrons and protons by an intense electric field (see Figure 2.2 top).  
 1127 The resulting protons leave the metal cylinder towards a radio frequency quadrupole  
 1128 (RFQ) that focus the beam, accelerates the protons and creates the packets of protons  
 1129 called bunches. In the RFQ, an electric field is generated by a RF wave at a frequency  
 1130 that matches the resonance frequency of the cavity where the electrodes are contained.  
 1131 The beam of protons traveling on the RFQ axis experiences an alternating electric  
 1132 field gradient that generates the focusing forces.

1133 In order to accelerate the protons, a longitudinal time-varying electric field com-  
 1134 ponent is added to the system; it is done by giving the electrodes a sine-like profile as  
 1135 shown in Figure 2.2 bottom. By matching the speed and phase of the protons with  
 1136 the longitudinal electric field the bunching is performed; protons synchronized with

1137 the RFQ (synchronous protons) do not feel an accelerating force, but those protons in  
 1138 the beam that have more (or less) energy than the synchronous proton (asynchronous  
 1139 protons) will feel a decelerating (accelerating) force; therefore, asynchronous protons  
 1140 will oscillate around the synchronous ones forming bunches of protons [63]. From the  
 1141 RFQ protons emerge with energy 750 keV in bunches of about  $1.15 \times 10^{11}$  protons [64].

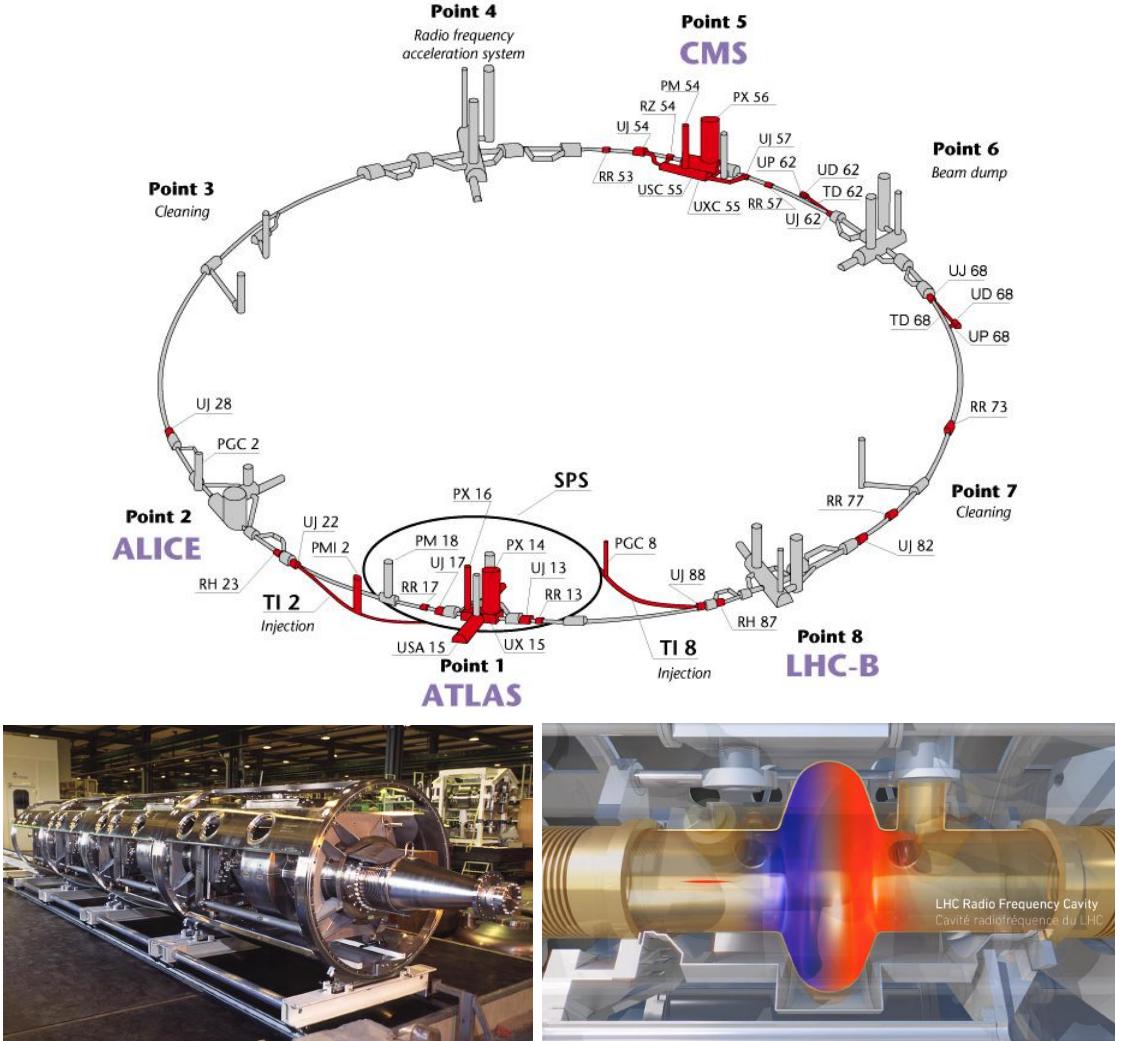


**Figure 2.3:** Left: drawing of the LINAC2 accelerating system at CERN. Electric fields generated by radio frequency (RF) create acceleration and deceleration zones inside the cavity; deceleration zones are blocked by drift tubes where quadrupole magnets focus the proton beam. Right: picture of a real RF cavity [67].

1142 Proton bunches coming from the RFQ go to the linear accelerator 2 (LINAC2)  
 1143 where they are accelerated to reach 50 MeV energy. In the LINAC2 stage, acceleration  
 1144 is performed using electric fields generated by radio frequency which create zones  
 1145 of acceleration and deceleration as shown in Figure 2.3. In the deceleration zones,  
 1146 the electric field is blocked using drift tubes where protons are free to drift while  
 1147 quadrupole magnets focus the beam.

1148 The beam coming from LINAC2 is injected into the proton synchrotron booster  
 1149 (PSB) to reach 1.4 GeV in energy. The next acceleration is provided at the proton  
 1150 synchrotron (PS) up to 26 GeV, followed by the injection into the super proton  
 1151 synchrotron (SPS) where protons are accelerated to 450 GeV. Finally, protons are  
 1152 injected into the LHC where they are accelerated to the target energy of 6.5 TeV.

1153 PSB, PS, SPS and LHC accelerate protons using the same RF acceleration tech-  
 1154 nique described before.



**Figure 2.4:** Top: LHC layout. The red zones indicate the infrastructure additions to the LEP installations, built to accommodate the ATLAS and CMS experiments which exceed the size of the former experiments located there [62]. Bottom: LHC RF cavities. A module (left picture) accommodates 4 cavities, each like the one in the right drawing, that accelerate protons and preserve the bunch structure of the beam. The color gradient pattern represents the strength of the electric field inside the cavity; red zone corresponds to the maximum of the oscillation electric field while the blue zone corresponds to the minimum. [66, 68]

1155        The LHC has a system of 16 RF cavities located in the so-called point 4, as  
 1156 shown in Figure 2.4 top, tuned at a frequency of 400 MHz. The bottom side of  
 1157 Figure 2.4 shows a picture of a RF module composed of 4 RF cavities working in a  
 1158 superconducting state at 4.5 K; also, a representation of the accelerating electric field

that accelerates the protons in the bunch is shown. The maximum of the oscillating electric field (red region) picks the proton bunches at the entrance of the cavity and keeps accelerating them through the whole cavity. The protons are carefully timed so that in addition to the acceleration effect the bunch structure of the beam is preserved.

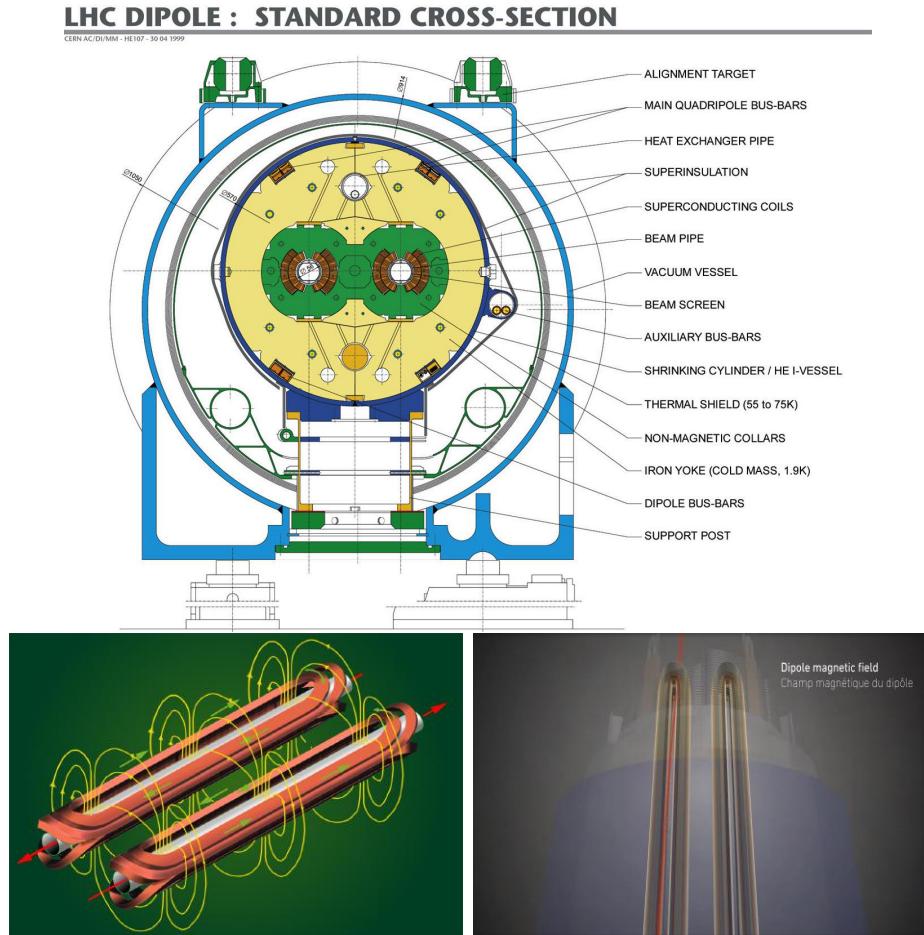
While protons are accelerated in one section of the LHC ring, where the RF cavities are located, in the rest of their path they have to be kept in the curved trajectory defined by the LHC ring. Technically, LHC is not a perfect circle; RF, injection, beam dumping, beam cleaning and sections before and after the experimental points where protons collide are all straight sections. In total, there are 8 arcs 2.45 km long each and 8 straight sections 545 m long each. In order to curve the proton's trajectory in the arc sections, superconducting dipole magnets are used.

Inside the LHC ring, there are two proton beams traveling in opposite directions in two separated beam pipes; the beam pipes are kept at ultra-high vacuum ( $\sim 10^{-9}$  Pa) to ensure that there are no particles that interact with the proton beams. The superconducting dipole magnets used in LHC are made of a NbTi alloy, capable of transporting currents of about 12000 A when cooled at a temperature below 2K using liquid helium (see Figure 2.5).

Protons in the arc sections of LHC feel a centripetal force exerted by the dipole magnets; the magnitude of magnetic field needed to keep the protons in the LHC curved trayectomy can be found assuming that protons travel at  $v \approx c$ , using the standard values for proton mass and charge and the LHC radius, as

$$F_m = \frac{mv^2}{r} = qBv \rightarrow B = 8.33T \quad (2.1)$$

which is about 100000 times the Earth's magnetic field. A representation of the



**Figure 2.5:** Top: LHC dipole magnet transverse view; cooling, shielding and mechanical support are indicated. Bottom left: Magnetic field generated by the dipole magnets; note that the direction of the field inside one beam pipe is opposite with respect to the other beam pipe which guarantee that both proton beams are curved in the same direction towards the center of the ring. The effect of the dipole magnetic field on the proton beam is represented on the bottom right side [66, 69, 70].

1182 magnetic field generated by the dipole magnets is shown on the bottom left side of  
 1183 Figure 2.5. The bending effect of the magnetic field on the proton beam is shown on  
 1184 the bottom right side of Figure 2.5. Note that the dipole magnets are not curved;  
 1185 the arc section of the LHC ring is composed of straight dipole magnets of about 15  
 1186 m. In total there are 1232 dipole magnets along the LHC ring.

1187 In addition to the bending of the beam trajectory, the beam has to be focused. The

focusing is performed by quadrupole magnets installed in a different straight section; in total 858 quadrupole magnets are installed along the LHC ring. Other effects like electromagnetic interaction among bunches, interaction with electron clouds from the beam pipe, the gravitational force on the protons, differences in energy among protons in the same bunch, among others, are corrected using sextupole and other magnetic multipoles.

The two proton beams inside the LHC ring are made of bunches with a cylindrical shape of about 7.5 cm long and about 1 mm in diameter; when bunches are close to the interaction point (IP), the beam is focused up to a diameter of about 16  $\mu\text{m}$  in order to maximize the probability of collisions between protons. The number of collisions per second is proportional to the cross section of the bunches with the *luminosity* ( $L$ ) as the proportionality factor, thus, the luminosity can be calculated using

$$L = fn \frac{N_1 N_2}{4\pi\sigma_x\sigma_y} \quad (2.2)$$

where  $f$  is the revolution frequency,  $n$  is the number of bunches per beam,  $N_1$  and  $N_2$  are the numbers of protons per bunch,  $\sigma_x$  and  $\sigma_y$  are the gaussian transverse sizes of the bunches. With the expected parameters, the LHC expected luminosity is about

$$f = \frac{v}{2\pi r_{LHC}} \approx \frac{3 \times 10^8 \text{ m/s}}{27 \text{ km}} \approx 11.1 \text{ kHz},$$

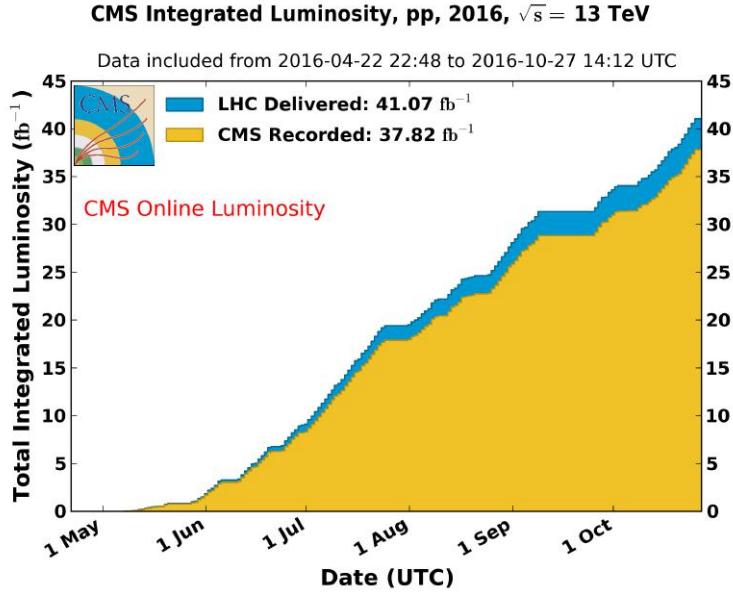
$$n = 2808$$

$$N_1 = N_2 \sim 1.5 \times 10^{11}$$

$$\sigma_x = \sigma_y = 16 \mu\text{m}$$

1203

$$L = 1.28 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1} = 1.28 \times 10^{-5} \text{ fb}^{-1} \text{ s}^{-1} \quad (2.3)$$



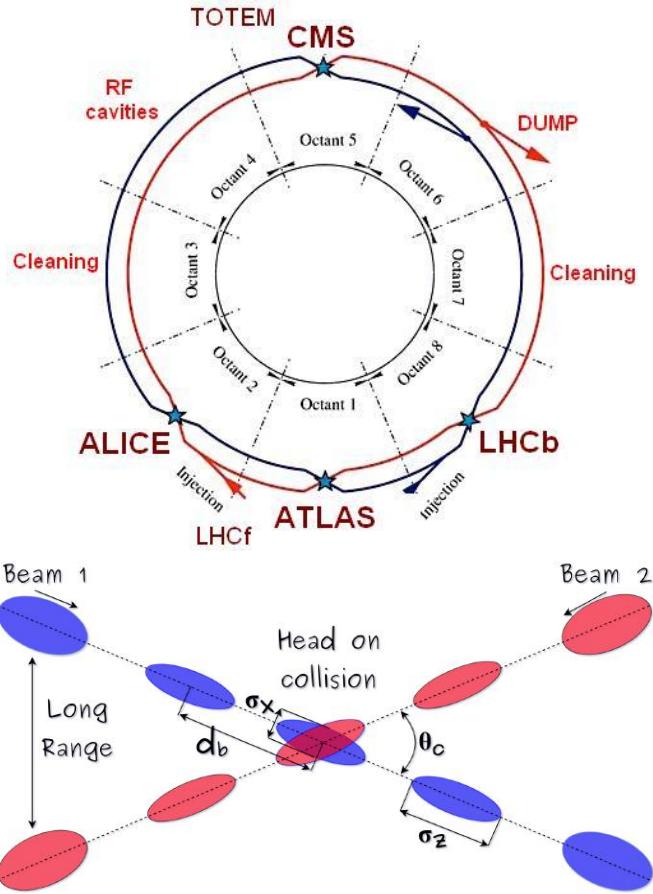
**Figure 2.6:** Integrated luminosity delivered by LHC and recorded by CMS during 2016. The difference between the delivered and the recorded luminosity is due to fails and issues occurred during the data taking in the CMS experiment [71].

1204        Luminosity is a fundamental aspect of LHC given that the bigger luminosity the  
 1205        bigger number of collisions, which means that for processes with a very small cross  
 1206        section the number of expected occurrences is increased and so the chances of being  
 1207        detected. The integrated luminosity, collected by the CMS experiment during 2016  
 1208        is shown in Figure 2.6; the data analyzed in this thesis corresponds to an integrated  
 1209        luminosity of  $35.9 \text{ fb}^{-1}$  at a center of mass-energy  $\sqrt{s} = 13 \text{ TeV}$ .

1210        One way to increase  $L$  is increasing the number of bunches in the beam. Cur-  
 1211        rently, the separation between two consecutive bunches in the beam is 7.5 m which  
 1212        corresponds to a time separation of 25 ns. In the full LHC ring the allowed number  
 1213        of bunches is  $n = 27\text{km}/7.5\text{m} = 3600$ ; however, there are some gaps in the bunch pat-  
 1214        tern intended for preparing the dumping and injection of the beam, thus, the proton  
 1215        beams are composed of 2808 bunches.

1216        Once the proton beams reach the desired energy, they are brought to cross each

1217 other producing  $pp$  collisions. The bunch crossing happens in precise places where  
 1218 the four LHC experiments are located, as seen in the top of Figure 2.7. In 2008  $pp$   
 1219 collisions of  $\sqrt{s} = 7$  TeV were performed; the energy was increased to 8 TeV in 2012  
 1220 and to 13 TeV in 2015.



**Figure 2.7:** Top: LHC interaction points. Bunch crossing occurs where the LHC experiments are located [72]. Sections indicated as cleaning are dedicated to collimate the beam in order to protect the LHC ring from collisions with protons in very spreaded bunches. Bottom: bunch crossing scheme. Since the bunch crossing is not perfectly head-on, the luminosity is reduced in a factor of 17%; adapted from Reference [86].

1221 The CMS and ATLAS experiments are multi-purpose experiments, hence, they  
 1222 are enabled to explore physics in any of the LHC collision modes. LHCb experiment  
 1223 is optimized to explore bottom quark physics, while ALICE is optimized for heavy

1224 ion collisions searches; TOTEM and LHCf are dedicated to forward physics studies;  
 1225 MoEDAL (not indicated in the Figure) is intended for monopole or massive pseudo  
 1226 stable particles searches.

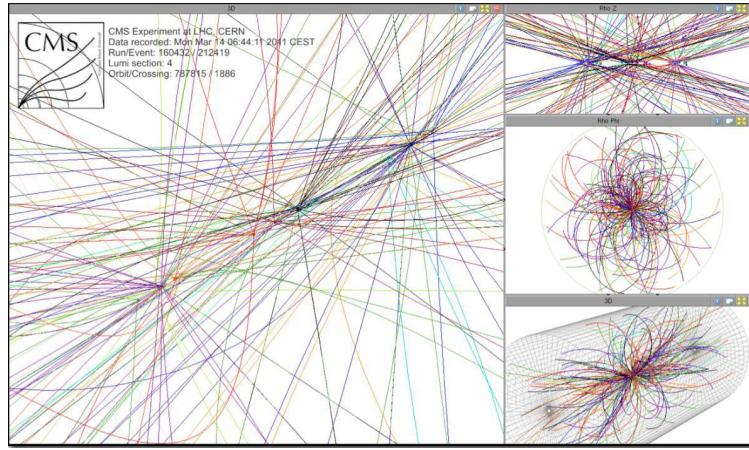
1227 At the IP there are two interesting details that need to be addressed. The first  
 1228 one is that the bunch crossing does not occur head-on but at a small crossing angle  $\theta_c$   
 1229 (280  $\mu$ rad in CMS and ATLAS) as shown in the bottom side of Figure 2.7, affecting  
 1230 the overlapping between bunches; the consequence is a reduction of about 17% in  
 1231 the luminosity (represented by a factor not included in eqn. 2.2). The second one  
 1232 is the occurrence of multiple  $pp$  collisions in the same bunch crossing; this effect is  
 1233 called *pileup* (PU). A fairly simple estimation of the PU follows from estimating the  
 1234 probability of collision between two protons, one from each of the bunches in the  
 1235 course of collision; it depends roughly on the ratio of proton size and the cross section  
 1236 of the bunch in the IP, i.e.,

$$P(pp\text{-}collision) \sim \frac{d_{proton}^2}{\sigma_x \sigma_y} = \frac{(1\text{fm})^2}{(16\mu\text{m})^2} \sim 4 \times 10^{-21} \quad (2.4)$$

1237 however, there are  $N = 1.15 \times 10^{11}$  protons in a bunch, thus the estimated number of  
 1238 collisions in a bunch crossing is

$$PU = N^2 * P(pp\text{-}collision) \sim 50pp \text{ collision per bunch crossing}, \quad (2.5)$$

1239 about 20 of which are inelastic. A multiple  $pp$  collision event in a bunch crossing at  
 1240 CMS is shown in Figure 2.8.

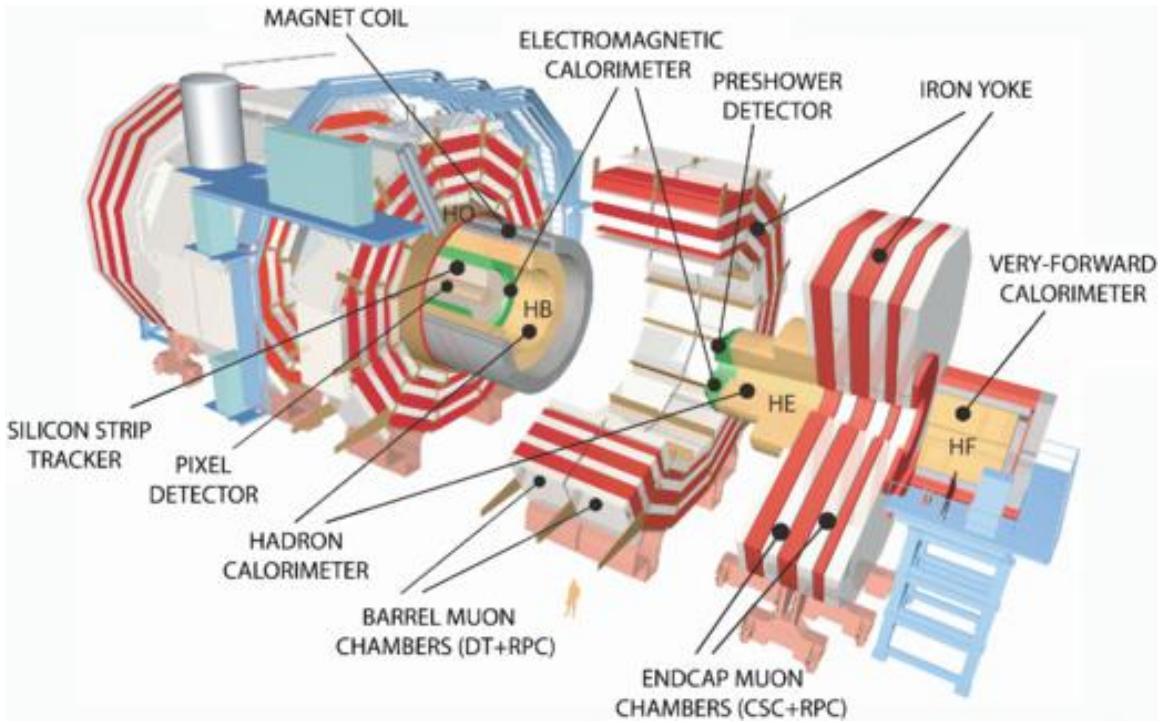


**Figure 2.8:** Multiple  $pp$  collision bunch crossing at CMS. [73].

## 1241 2.3 The CMS experiment

1242 CMS is a general-purpose detector designed to conduct research in a wide range  
 1243 of physics from the standard model to new physics like extra dimensions and dark  
 1244 matter. Located at Point 5 in the LHC layout as shown in Figure 2.4, CMS is  
 1245 composed of several detection systems distributed in a cylindrical structure; in total,  
 1246 CMS weights about 12500 tons in a very compact 21.6 m long and 14.6 m diameter  
 1247 cylinder. It was built in 15 separate sections at the ground level and lowered to the  
 1248 cavern individually to be assembled. A complete and detailed description of the CMS  
 1249 detector and its components is given in Reference [74] on which this section is based.  
 1250 Figure 2.9 shows the layout of the CMS detector. The detection system is composed  
 1251 of (from the innermost to the outermost)

- 1252     • Pixel detector.
- 1253     • Silicon strip tracker.
- 1254     • Preshower detector.
- 1255     • Electromagnetic calorimeter.



**Figure 2.9:** Layout of the CMS detector. The several subdetectors are indicated. The central region of the detector is referred as the barrel section while the endcaps are referred as the forward sections. [75].

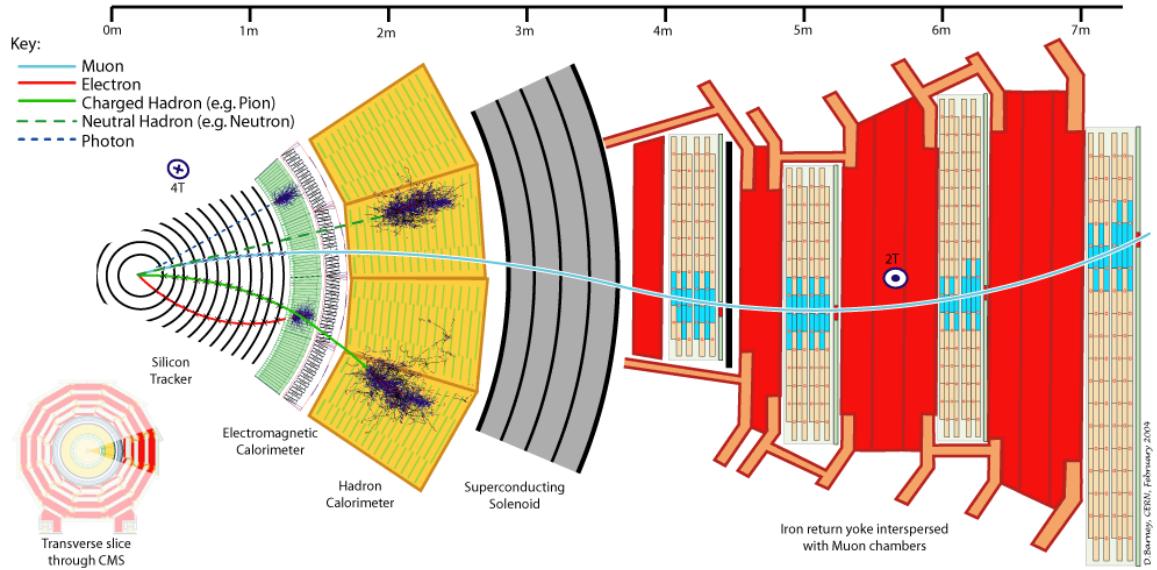
1256        • Hadronic calorimeter.

1257        • Muon chambers (barrel and endcap)

1258        The central region of the detector is commonly referred as the barrel section while  
 1259        the endcaps are referred as the forward sections of the detector; thus, each subdetector  
 1260        is composed of a barrel section and a forward section.

1261        When a  $pp$  collision happens inside the CMS detector, many different particles are  
 1262        produced, but only some of them live long enough to be detected; they are electrons,  
 1263        photons, pions, kaons, protons, neutrons and muons; neutrinos are not detected by  
 1264        the CMS detector. Thus, the CMS detector was designed to detect those particles and  
 1265        measure their properties. Figure 2.10 shows a transverse slice of the CMS detector.  
 1266        The silicon tracker (pixel detector + strip tracker) is capable to register the track of

1267 the charged particles traversing it, while calorimeters (electromagnetic and hadronic)  
 1268 measure the energy of the particles that are absorbed by their materials. Considering  
 1269 the detectable particles, mentioned above, emerging from the IP, a basic description  
 1270 of the detection process is as follows.



**Figure 2.10:** CMS detector transverse slice [76].

1271 A muon emerging from the IP, will create a track on the silicon tracker and on  
 1272 the muon chambers. The design of the CMS detector is driven by the requirements  
 1273 on the identification, momentum resolution and unambiguous charge determination  
 1274 of the muons; therefore, a large bending power is provided by the solenoid magnet  
 1275 made of superconducting cable capable of generating a 3.8 T magnetic field. The  
 1276 muon track is bent twice since the magnetic field inside the solenoid is directed along  
 1277 the  $z$ -direction but outside its direction is reversed. Muons interact very weakly with  
 1278 the calorimeters, therefore, it is not absorbed but escape away from the detector.

1279 An electron emerging from the IP will create a track along the tracker which will  
 1280 be bent due to the presence of the magnetic field, later, it will be absorbed in the  
 1281 electromagnetic calorimeter where its energy is measured.

1282        A photon will not leave a track because it is neutral, but it will be absorbed in  
 1283        the electromagnetic calorimeter.

1284        A neutral hadron, like the neutron, will not leave a track either but it will lose a  
 1285        small amount of its energy during its passage through the electromagnetic calorimeter  
 1286        and then it will be absorbed in the hadron calorimeter depositing the rest of its energy.

1287        A charged hadron, like the proton or  $\pi^\pm$ , will leave a curved track on the silicon  
 1288        tracker, some of its energy in the electromagnetic calorimeter and finally will be  
 1289        absorbed in the hadronic calorimeter.

1290        A more detailed description of each detection system will be presented in the  
 1291        following sections.

### 1292        2.3.1 CMS coordinate system

1293        The coordinate system used by CMS is centered on the geometrical center of the  
 1294        detector which is the nominal IP as shown in Figure 2.11<sup>1</sup>. The  $z$ -axis is parallel  
 1295        to the beam direction, while the  $Y$ -axis pointing vertically upward, and the  $X$ -axis  
 1296        pointing radially inward toward the center of the LHC.

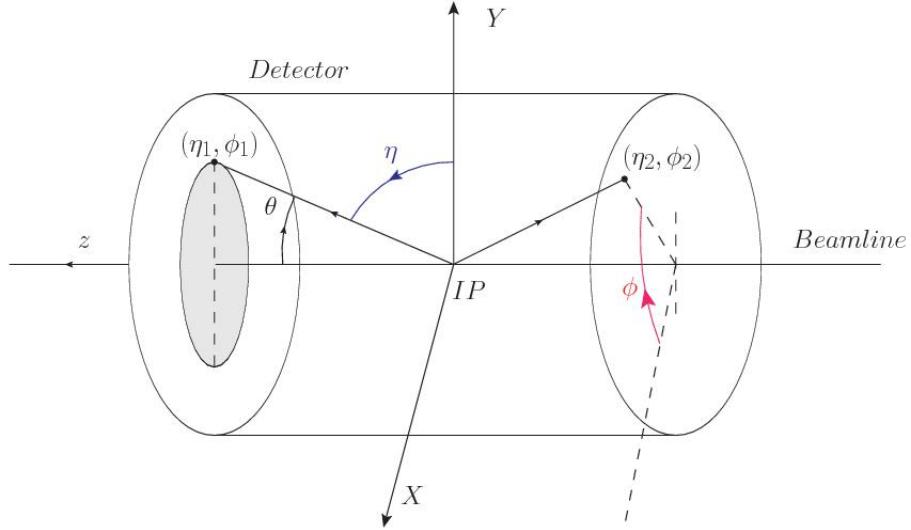
1297        In addition to the common cartesian and cylindrical coordinate systems, two co-  
 1298        ordinates are of particular utility in particle physics: rapidity ( $y$ ) and pseudorapidity  
 1299        ( $\eta$ ), defined in connection to the polar angle  $\theta$ , energy and longitudinal momentum  
 1300        component (momentum along the  $z$ -axis) according to

$$y = \frac{1}{2} \ln \frac{E + p_z}{E - p_z} \quad \eta = -\ln \left( \tan \frac{\theta}{2} \right) \quad (2.6)$$

1301        Rapidity is related to the angle between the  $XY$ -plane and the direction in which  
 1302        the products of a collision are emitted; it has the nice property that the difference

---

<sup>1</sup> Not all the  $pp$  interaction occur at the nominal IP because of the bunch lenght, therefore, each  $pp$  collision has its own IP location



**Figure 2.11:** CMS detector coordinate system.

1303 between the rapidities of two particles is invariant with respect to Lorentz boosts  
 1304 along the  $z$ -axis, hence, data analysis becomes more simple when based on rapid-  
 1305 ity; however, it is not simple to measure the rapidity of highly relativistic particles,  
 1306 as those produced after  $pp$  collisions. Under the highly relativistic motion approxi-  
 1307 mation,  $y$  can be rewritten in terms of the polar angle, concluding that rapidity is  
 1308 approximately equal to the pseudorapidity defined above, i.e.,  $y \approx \eta$ . Note that  $\eta$   
 1309 is easier to measure than  $y$  given the direct relationship between the former and the  
 1310 polar angle.

1311 The angular distance between two objects in the detector ( $\Delta R$ ) is commonly used  
 1312 to judge the isolation of those object; it is defined in terms of their coordinates  $(\eta_1, \phi_1)$ ,  
 1313  $(\eta_2, \phi_2)$  as

$$\Delta R = \sqrt{(\Delta\eta)^2 - (\Delta\phi)^2} \quad (2.7)$$

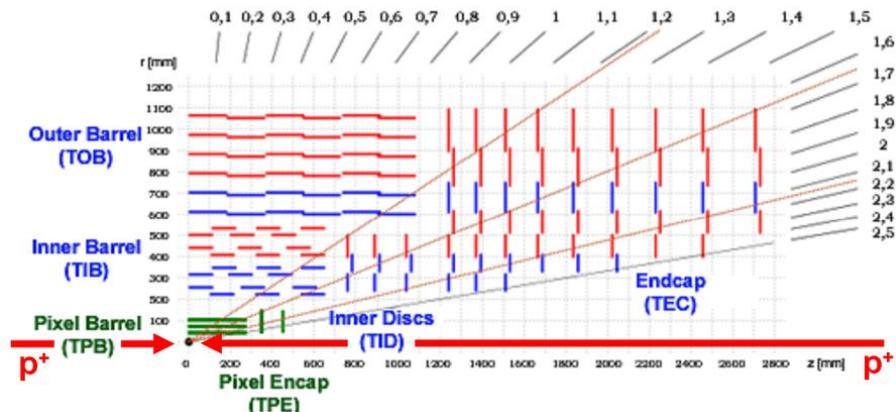
### 1314 2.3.2 Tracking system

1315 The CMS tracking system is designed to provide a precise measurement of the trajectories (*track*) followed by the charged particles created after the  $pp$  collisions; also, the  
 1316 precise reconstruction of the primary and secondary origins of the tracks (*vertices*) is  
 1317 expected in an environment where, each 25 ns, the bunch crossing produces about 20  
 1318 inelastic collisions and about 1000 particles.  
 1319

1320 Physics requirements guiding the tracking system performance include the precise characterization of events involving gauge bosons, W and Z, and their leptonic  
 1321 decays for which an efficient isolated lepton and photon reconstruction is of capital  
 1322 importance, given that isolation is required to suppress background events to a level  
 1323 that allows observations of interesting processes like Higgs boson decays or beyond  
 1324 SM events.

1326 The ability to identify and reconstruct  $b$ -jets and B-hadrons within these jets is also  
 1327 a fundamental requirement, achieved through the ability to reconstruct accurately  
 1328 displaced vertices, given that  $b$ -jets are part of the signature of top quark physics, like  
 1329 the one treated in this thesis.

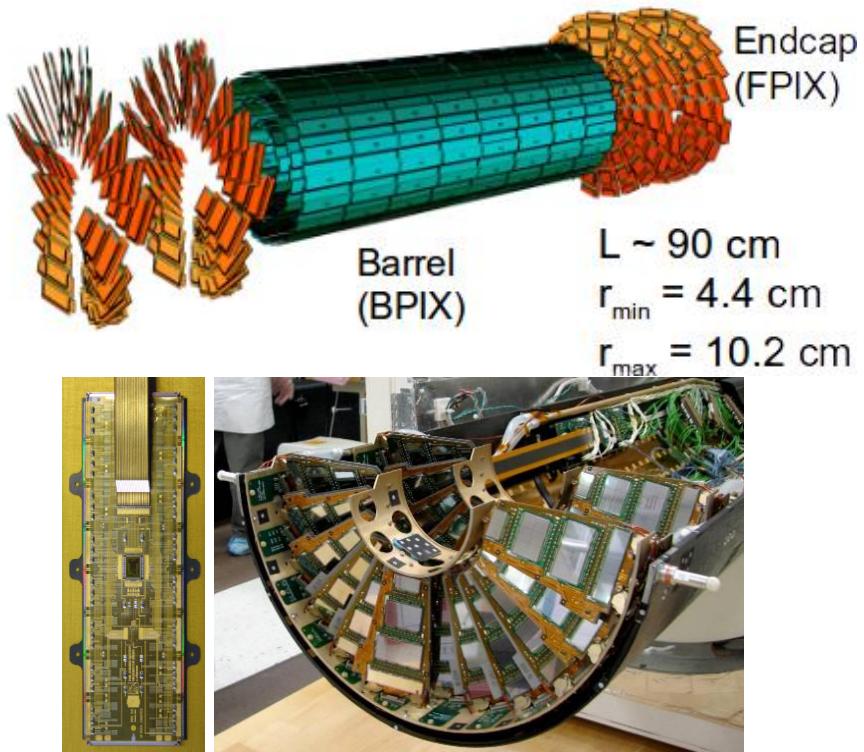
1330 An schematic view of the CMS tracking system is shown in Figure 2.12



**Figure 2.12:** CMS tracking system schematic view [78].

1331 In order to satisfy these performance requirements, the tracking system uses two  
 1332 different detector subsystems arranged in concentric cylindrical volumes, the pixel  
 1333 detector and the silicon strip tracker; the pixel detector is located in the high particle  
 1334 density region ( $r < 20\text{cm}$ ) while the silicon strip tracker is located in the medium and  
 1335 lower particle density regions  $20\text{cm} < r < 116\text{cm}$ .

1336 **Pixel detector**



**Figure 2.13:** CMS pixel detector. Top: schematic view; Bottom: pictures of a barrel(BPIX) module(left) and forward modules(right) [74].

1337 The pixel detector was replaced during the 2016-2017 extended year-end technical  
 1338 stop, due to the increasingly challenging operating conditions like the higher particle  
 1339 flux and more radiation harsh environment, among others. The new one is responding  
 1340 as expected, reinforcing its crucial role in the successful way to fulfill the new LHC

1341 physics objectives after the discovery of the Higgs boson. Since the data sets used  
 1342 in this thesis were produced using the previous version of the pixel detector, it will  
 1343 be the subject of the description in this section. The last chapter of this thesis is  
 1344 dedicated to describe my contribution to the *Forward Pixel Phase 1 upgrade*.

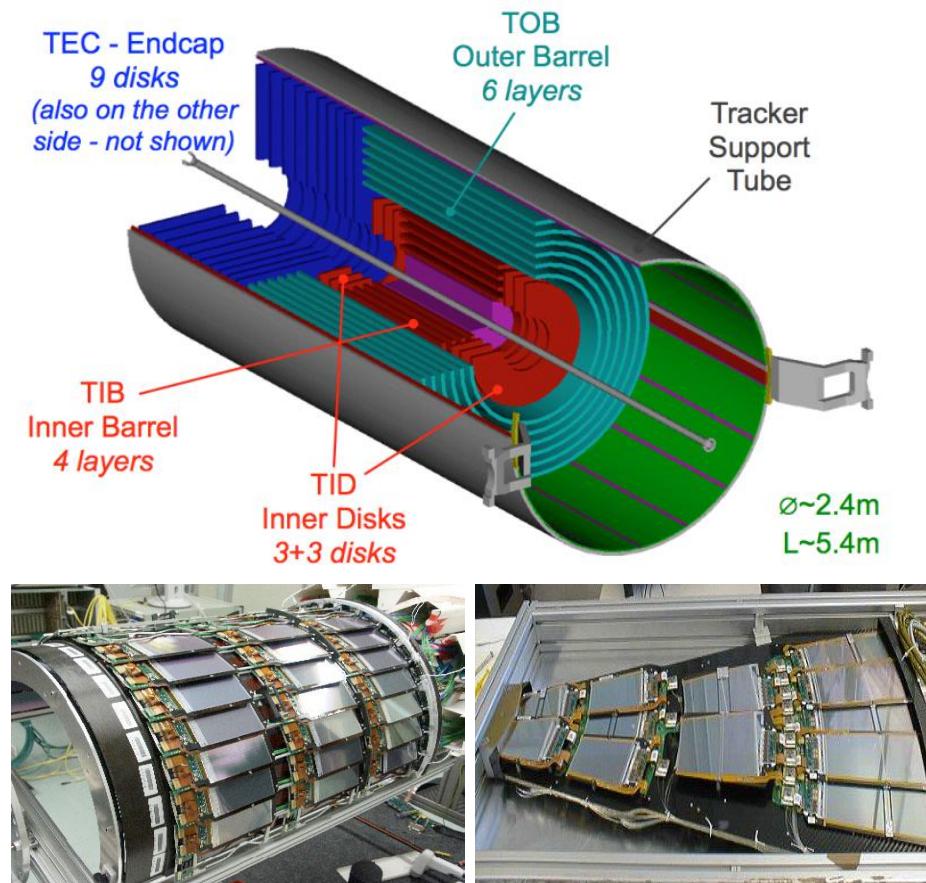
1345 The pixel detector was composed of 1440 silicon pixel detector modules organized  
 1346 in three-barrel layers in the central region (BPix) and two disks in the forward region  
 1347 (FPix) as shown in the top side of Figure 2.13; it was designed to record efficiently  
 1348 and with high precision, up to  $20\mu\text{m}$  in the  $XY$ -plane and  $20\mu\text{m}$  in the  $z$ -direction,  
 1349 the first three space-points (*hits*) nearest to the IP region in the range  $|\eta| \leq 2.5$ . The  
 1350 first barrel layer was located at a radius of 44 mm from the beamline, while the third  
 1351 layer was located at a radius of 102 mm, closer to the strip tracker inner barrel layer  
 1352 (see Section 2.3.3) in order to reduce the rate of fake tracks. The high granularity of  
 1353 the detector is represented in its about 66 Mpixels, each of size  $100 \times 150\mu\text{m}^2$ . The  
 1354 transverse momentum resolution of tracks can be measured with a resolution of 1-2%  
 1355 for muons of  $p_T = 100$  GeV.

1356 A charged particle passing through the pixel sensors produce ionization in them,  
 1357 giving energy for electrons to be removed from the silicon atoms, hence, creating  
 1358 electron-hole pairs. The collection of charges in the pixels generates an electrical  
 1359 signal that is read out by an electronic readout chip (ROC); each pixel has its own  
 1360 electronics which amplifies the signal. Combining the signal from the pixels activated  
 1361 by a traversing particle in the several layers of the detector allows one to reconstruct  
 1362 the particle's trajectory in 3D.

1363 Commonly, the charge produced by traversing of a particle is collected by and  
 1364 shared among several pixels; by interpolating between pixels, the spatial resolution  
 1365 is improved. In the barrel section the charge sharing in the  $r\phi$ -plane is due to the  
 1366 Lorentz effect. In the forward pixels the charge sharing is enhanced by arranging the

1367 blades in the turbine-like layout as shown in Figure 2.13 bottom left.

### 1368 2.3.3 Silicon strip tracker



**Figure 2.14:** Top: CMS Silicon Strip Tracker (SST) schematic view. The SST is composed of the tracker inner barrel (TIB), the tracker inner disks (TID), the tracker outer barrel (TOB) and the tracker endcaps (TEC). Each part is made of silicon strip modules; the modules in blue represent two modules mounted back-to-back and rotated in the plane of the module by a stereo angle of 120 mrad in order to provide a 3-D reconstruction of the hit positions. Bottom: pictures of the TIB (left) and TEC (right) modules [80–82].

1369 The silicon strip tracker (SST) is the second stage in the CMS tracking system.

1370 The top side of Figure 2.14 shows a schematic of the SST. The inner tracker region is

1371 composed of the tracker inner barrel (TIB) and the tracker inner disks (TID) covering

1372 the region  $r < 55$  cm and  $|z| < 118$  cm. The TIB is composed of 4 layers while the TID

1373 is composed of 3 disks at each end. The silicon sensors in the inner tracker are 320  
 1374  $\mu\text{m}$  thick, providing a resolution of about 13-38  $\mu\text{m}$  in the  $r\phi$  position measurement.

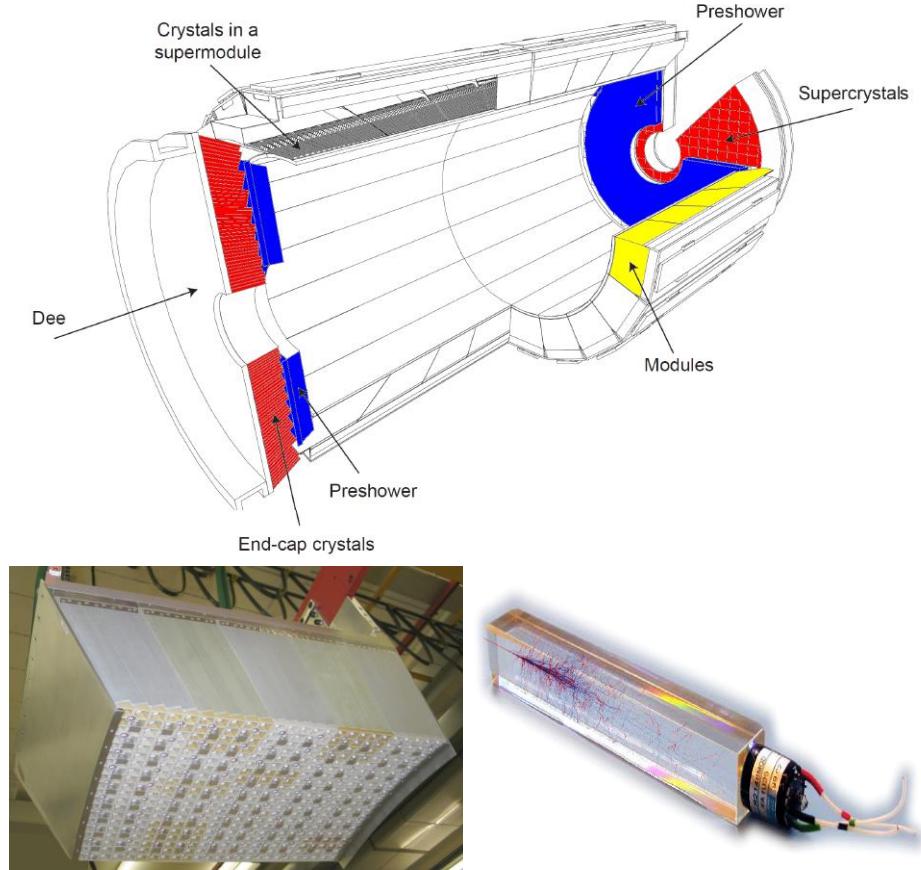
1375       The modules indicated in blue in the schematic view of Figure 2.14 are two mod-  
 1376 ules mounted back-to-back and rotated in the plane of the module by a *stereo* angle  
 1377 of 100 mrad; the hits from these two modules, known as *stereo hits*, are combined to  
 1378 provide a measurement of the second coordinate ( $z$  in the barrel and  $r$  on the disks)  
 1379 allowing the reconstruction of hit positions in 3-D.

1380       The outer tracker region is composed of the tracker outer barrel (TOB) and the  
 1381 tracker endcaps (TEC). The six layers of the TOB offer coverage in the region  $r > 55$   
 1382 cm and  $|z| < 118$  cm, while the 9 disks of the TEC cover the region  $124 < |z| < 282$   
 1383 cm. The resolution offered by the outer tracker is about 13-38  $\mu\text{m}$  in the  $r\phi$  position  
 1384 measurement. The inner four TEC disks use silicon sensors 320  $\mu\text{m}$  thick; those in  
 1385 the TOB and the outer three TEC disks use silicon sensors of 500  $\mu\text{m}$  thickness. The  
 1386 silicon strips run parallel to the  $z$ -axis and the distance between strips varies from 80  
 1387  $\mu\text{m}$  in the inner TIB layers to 183  $\mu\text{m}$  in the inner TOB layers; in the endcaps the  
 1388 wedge-shaped sensors with radial strips, whose pitch range between 81  $\mu\text{m}$  at small  
 1389 radii and 205  $\mu\text{m}$  at large radii.

1390       The whole SST has 15148 silicon modules, 9.3 million silicon strips and cover a  
 1391 total active area of about 198  $\text{m}^2$ .

### 1392   **2.3.4 Electromagnetic calorimeter**

1393 The CMS electromagnetic calorimeter (ECAL) is designed to measure the energy of  
 1394 electrons and photons. It is composed of 75848 lead tungstate crystals which have a  
 1395 short radiation length (0.89 cm) and fast response, since 80% of the light is emitted  
 1396 within 25 ns; however, they are combined with Avalanche photodiodes (APDs) as



**Figure 2.15:** Top: CMS ECAL schematic view. Bottom: Module equipped with the crystals (left); ECAL crystal(right) with an artistic representation of an electromagnetic shower [74].

1397 photodetectors given that crystals themselves have a low light yield ( $30\gamma/\text{MeV}$ ). A  
 1398 schematic view of the ECAL is shown in Figure 2.15.

1399 Energy is measured when electrons and photons are absorbed by the crystals  
 1400 which generates an electromagnetic *shower*, as seen in bottom right picture of the  
 1401 Figure 2.15; the shower is seen as a *cluster* of energy which depending on the amount  
 1402 of energy deposited can involve several crystals. The ECAL barrel (EB) covers the  
 1403 region  $|\eta| < 1.479$ , using crystals of depth of 23 cm and  $2.2 \times 2.2 \text{ cm}^2$  transverse  
 1404 section; the ECAL endcap (EE) covers the region  $1.479 < |\eta| < 3.0$  using crystals of  
 1405 depth 22 cm and transverse section of  $2.86 \times 2.86 \text{ cm}^2$ ; the photodetectors used are

1406 vacuum phototriodes (VPTs). Each EE is divided in two structures called *Dees*.

1407 The preshower detector (ES) is installed in front of the EE and covers the region  
 1408  $1.653 < |\eta| < 2.6$ . The ES provides a precise measurement of the position of electro-  
 1409 magnetic showers, which allows to distinguish electrons and photon signals from  $\pi^0$   
 1410 decay signals. The ES is composed of a layer of lead radiators followed by a layer of  
 1411 silicon strip sensors. The lead radiators initiate electromagnetic showers when reached  
 1412 by photons and electrons, then, the strip sensors measure the deposited energy and  
 1413 the transverse shower profiles. The full ES thickness is 20 cm.

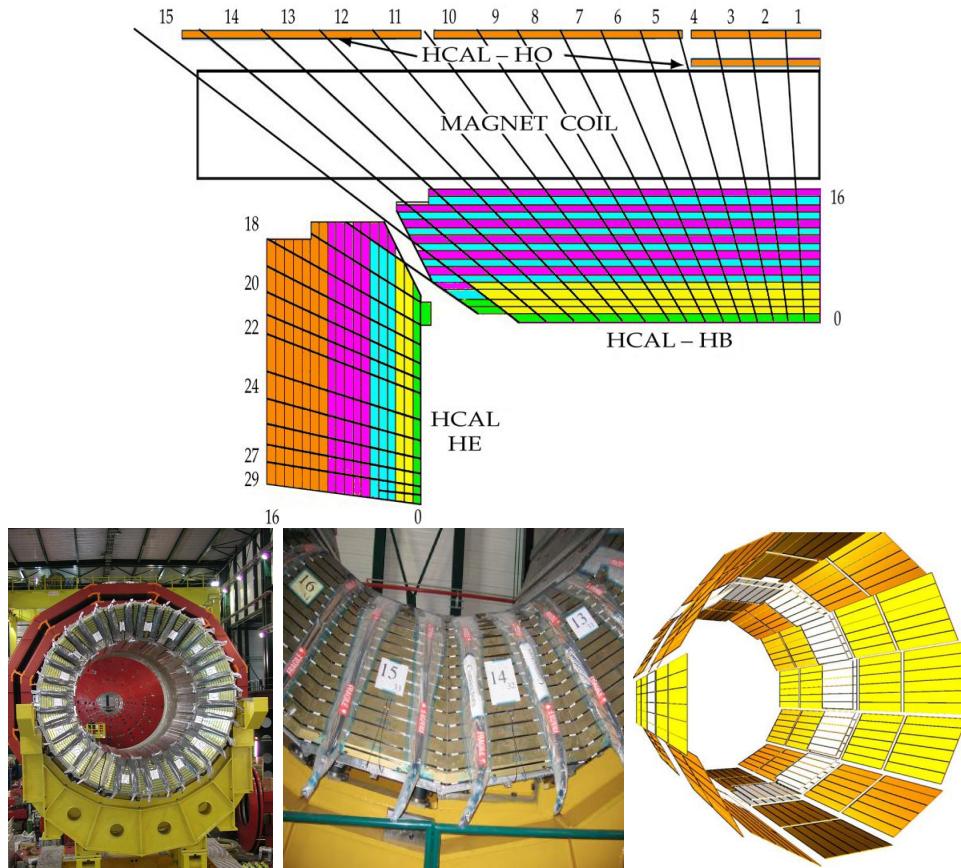
### 1414 2.3.5 Hadronic calorimeter

1415 Hadrons are not absorbed by the ECAL<sup>2</sup> but by the hadron calorimeter (HCAL),  
 1416 which is made of a combination of alternating brass absorber layers and silicon photo-  
 1417 multiplier(SiPM) layers; therefore, particles passing through the scintillator material  
 1418 produce showers, as in the ECAL, as a result of the inelastic scattering of the hadrons  
 1419 with the detector material. Since the particles are not absorbed in the scintillator,  
 1420 their energy is sampled; therefore the total energy is not measured but estimated from  
 1421 the energy clusters, which reduces the resolution of the detector. Brass was chosen  
 1422 as the absorber material due to its short interaction length ( $\lambda_I = 16.42\text{cm}$ ) and its  
 1423 non-magnetivity. Figure 2.16 shows a schematic view of the CMS HCAL.

1424 The HCAL is divided into four sections; the Hadron Barrel (HB), the Hadron  
 1425 Outer (HO), the Hadron Endcap (HE) and the Hadron Forward (HF) sections. The  
 1426 HB covers the region  $0 < |\eta| < 1.4$ , while the HE covers the region  $1.3 < |\eta| < 3.0$ .  
 1427 The HF, made of quartz fiber scintillator and steel as absorption material, covers the  
 1428 forward region  $3.0 < |\eta| < 5.2$ . Both the HB and HF are located inside the solenoid.  
 1429 The HO is placed outside the magnet as an additional layer of scintillators with the

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<sup>2</sup> Most hadrons are not absorbed, but few low-energy ones might be.

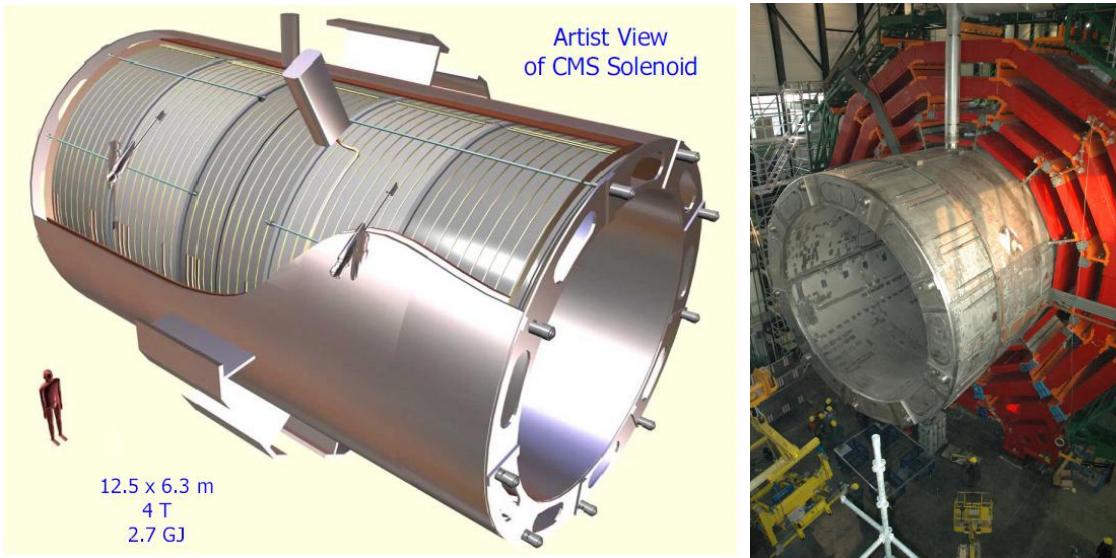


**Figure 2.16:** Top: CMS HCAL schematic view, the colors indicate the layers that are grouped into the same readout channels. Bottom: picture of a section of the HB; the absorber material is the golden region and scintillators are placed in between the absorber material (left and center). Schematic view of the HO (right). [83,84]

1430 purpose of measure the energy tails of particles passing through the HB and the  
 1431 magnet (see Figure 2.16 top and bottom right).

### 1432 **2.3.6 Superconducting solenoid magnet**

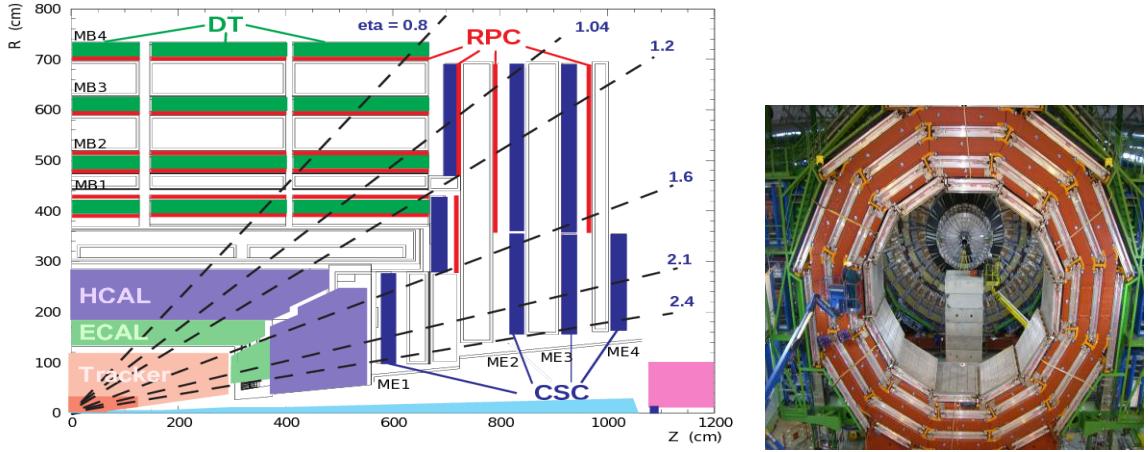
1433 The superconducting magnet installed in the CMS detector is designed to provide  
 1434 an intense and highly uniform magnetic field in the central part of the detector.  
 1435 In fact, the tracking system takes advantage of the bending power of the magnetic  
 1436 field to measure with precision the momentum of the particles that traverse it; the



**Figure 2.17:** Artistic representation of the CMS solenoid magnet(left). The magnet is supported on an iron yoke (right) which also serves as the house of the muon detector and as mechanical support for the whole CMS detector [77].

1437 unambiguous determination of the sign for high momentum muons was a driving  
 1438 principle during the design of the magnet. The magnet has a diameter of 6.3 m, a  
 1439 length of 12.5 m and a cold mass of 220 t; the generated magnetic field reaches a  
 1440 strength of 3.8T. Since it is made of Ni-Tb superconducting cable it has to operate at  
 1441 a temperature of 4.7 K by using a helium cryogenic system; the current circulating in  
 1442 the cables reaches 18800 A under normal running conditions. The left side of Figure  
 1443 2.17 shows an artistic view of the CMS magnet, while the right side shows a transverse  
 1444 view of the cold mass where the winding structure is visible.

1445 The yoke (see Figure 2.17), composed of 5 barrel wheels and 6 endcap disks made  
 1446 of iron, serves not only as the media for magnetic flux return but also provides housing  
 1447 for the muon detector system and structural stability to the full detector.



**Figure 2.18:** Left: CMS muon system schematic view; Right: one of the yoke rings with the muon DTs and RPCs installed; in the back it is possible to see the muon endcap [85].

### 1448 2.3.7 Muon system

1449 Muons are the only charged particles able to pass through all the CMS detector due  
 1450 to their low ionization energy loss; thus, muons can be separated easily from the  
 1451 high amount of particles produced in a  $pp$  collision. Also, muons are expected to be  
 1452 produced in the decay of several new particles; therefore, good detection of muons  
 1453 was one of the leading principles when designing the CMS detector.

1454 The CMS muon detection system (muon spectrometer) is embedded in the return  
 1455 yoke as seen in Figure 2.18. It is composed of three different detector types, the drift  
 1456 tube chambers (DT), cathode strip chambers (CSC), and resistive plate chambers  
 1457 (RPC); DT are located in the central region  $\eta < 1.2$  arranged in four layers of drift  
 1458 chambers filled with an Ar/CO<sub>2</sub> gas mixture.

1459 The muon endcaps are made of CSCs covering the region  $\eta < 2.4$  and filled with  
 1460 a mixture of Ar/CO<sub>2</sub>/CF<sub>4</sub>. The reason behind using a different detector type lies on  
 1461 the different conditions in the forward region like the higher muon rate and higher  
 1462 residual magnetic field compared to the central region.

1463 The third type of detector used in the muon system is a set of four disks of RPCs

1464 working in avalanche mode. The RPCs provide good spatial and time resolutions. The  
 1465 track of high- $p_T$  muon candidates is built combining information from the tracking  
 1466 system and the signal from up to six RPCs and four DT chambers.

1467 The muon tracks are reconstructed from the hits in the several layers of the muon  
 1468 system.

### 1469 **2.3.8 CMS trigger system**

1470 CMS expects  $pp$  collisions every 25 ns, i.e., an interaction rate of 40 MHz for which  
 1471 it is not possible to store the recorded data in full. In order to handle this high event  
 1472 rate data, an online event selection, known as triggering, is performed; triggering  
 1473 reduces the event rate to 100 Hz for storage and further offline analysis.

1474 The trigger system starts with a reduction of the event rate to 100 kHz in the  
 1475 so-called *the level 1 trigger* (L1). L1 is based on dedicated programmable hardware  
 1476 like Field Programmable Gate Arrays (FPGAs) and Application Specific Integrated  
 1477 Circuits (ASICs), partly located in the detector itself; another portion is located in  
 1478 the CMS underground cavern. Hit pattern information from the muon chambers  
 1479 and the energy deposits in the calorimeter are used to decide if an event is accepted  
 1480 or rejected, according to selection requirements previously defined, which reflect the  
 1481 interesting physics processes. Figure 2.19 shows the L1 trigger architecture.

1482 The second stage in the trigger system is called *the high-level trigger* (HLT); events  
 1483 accepted by L1 are passed to HLT in order to make an initial reconstruction of them.  
 1484 HLT is software based and runs on a dedicated server farm, using selection algorithms  
 1485 and high-level object definitions; the event rate at HLT is reduced to 100 Hz. The  
 1486 first HLT stage takes information from the muon detectors and the calorimeters to  
 1487 make the initial object reconstruction; in the next HLT stage, information from the

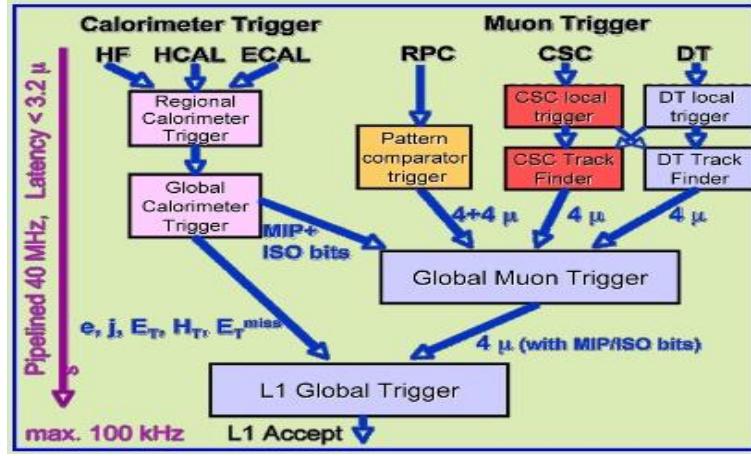


Figure 2.19: CMS Level-1 trigger architecture [86].

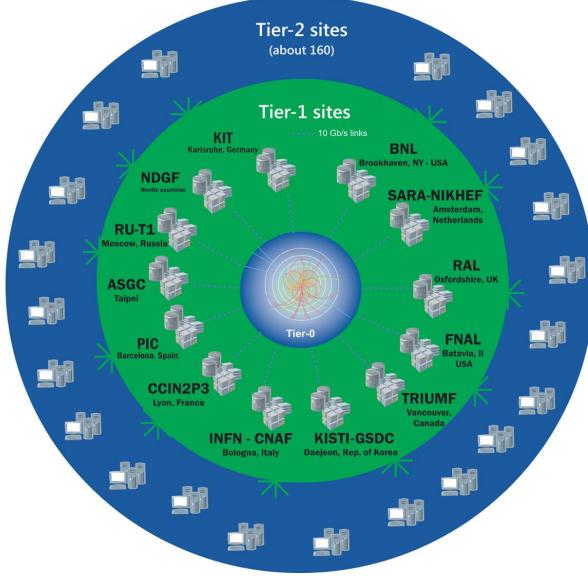
pixel and strip detectors is used to do first fast tracking and then full tracking online.  
 This initial object reconstruction is used in further steps of the trigger system.

Events and preliminary reconstructed physics objects from HLT are sent to be fully reconstructed at the CERN computing center known also as Tier-0 facility. Again, the pixel detector information provides high-quality seeds for the track reconstruction algorithm offline, primary vertex reconstruction, electron and photon identification, muon reconstruction,  $\tau$  identification, and b-tagging. After full reconstruction, data sets are made available for offline analyses.

### 2.3.9 CMS computing

Data coming from the experiment have to be stored and made available for further analysis; in order to cope with all the tasks implied in the offline data processing, like transfer, simulation, reconstruction and reprocessing, among others, a large computing power is required. The CMS computing system is based on the distributed architecture concept, where users of the system and physical computer centers are distributed worldwide and interconnected by high-speed networks.

The worldwide LHC computing grid (WLCG) is the mechanism used to provide



**Figure 2.20:** WLCG structure. The primary computer centers (Tier-0) are located at CERN (data center) and at the Wigner datacenter in Budapest. Tier-1 is composed of 13 centers and Tier-2 is composed of about 160 centers. [87].

1504 that distributed environment. WLCG is a tiered structure connecting computing  
 1505 centers around the world, which provides the necessary storage and computing facil-  
 1506 ties. The primary computing centers of the WLCG are located at the CERN and  
 1507 the Wigner datacenter in Budapest and are known as Tier-0 as shown in Figure 2.20.  
 1508 The main responsibilities for each tier level are [87]

- 1509     • **Tier-0:** initial reconstruction of recorded events and storage of the resulting  
 1510       datasets, the distribution of raw data to the Tier-1 centers.
- 1511     • **Tier-1:** provide storage capacity, support for the Grid, safe-keeping of a pro-  
 1512       portional share of raw and reconstructed data, large-scale reprocessing and safe-  
 1513       keeping of corresponding output, generation of simulated events, distribution  
 1514       of data to Tier 2s, safe-keeping of a share of simulated data produced at these  
 1515       Tier 2s.
- 1516     • **Tier-2:** store sufficient data and provide adequate computing power for spe-

1517       cific analysis tasks and proportional share of simulated event production and  
1518       reconstruction.

1519       Aside from the general computing strategy to manage the huge amount of data  
1520       produced by experiments, CMS uses a software framework to perform a variety of  
1521       processing, selection and analysis tasks. The central concept of the CMS data model  
1522       referred to as *event data model* (EDM) is the *Event*; therefore, an event is the unit  
1523       that contains the information from a single bunch crossing, any data derived from  
1524       that information like the reconstructed objects, and the details of the derivation.

1525       Events are passed as the input to the *physics modules* that obtain information  
1526       from them and create new information; for instance, *event data producers* add new  
1527       data into the events, *analyzers* produce an information summary from an event set,  
1528       *filters* perform selection and triggering.

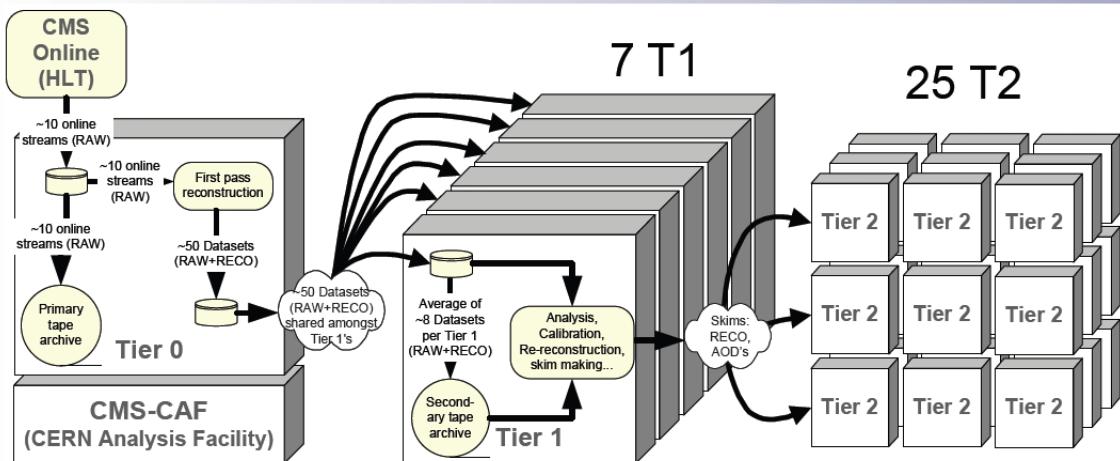
1529       CMS uses several event formats with different levels of detail and precision

1530       • **Raw format:** events in this format contain the full recorded information from  
1531       the detector as well as trigger decision and other metadata. An extended version  
1532       of raw data is used to store information from the CMS Monte Carlo simulation  
1533       tools (see Chapter 3). Raw data are stored permanently, occupying about  
1534       2MB/event

1535       • **RECO format:** events in this format correspond to raw data that have been  
1536       submitted to reconstruction algorithms like primary and secondary vertex re-  
1537       construction, particle ID, and track finding. RECO events contain physics ob-  
1538       jects and all the information used to reconstruct them; average size is about 0.5  
1539       MB/event.

- 1540     • **AOD format:** Analysis Object Data (AOD) is the data format used in the  
 1541       physics analyses given that it contains the parameters describing the high-level  
 1542       physics objects in addition to enough information to allow a kinematic refitting if  
 1543       needed. AOD events are filtered versions of the RECO events to which skimming  
 1544       or other filtering have been applied, hence AOD events are subsets of RECO  
 1545       events. Requires about 100 kB/event.
- 1546     • **Non-event data** are data needed to interpret and reconstruct events. Some  
 1547       of the non-event data used by CMS contains information about the detector  
 1548       contraction and condition data like calibrations, alignment, and detector status.

1549     Figure 2.21 shows the data flow scheme between CMS detector and tiers.



**Figure 2.21:** Data flow from CMS detector through tiers.

1550     The whole collection of software built as a framework is referred to as *CMSSW*. This  
 1551       framework provides the services needed by the simulation, calibration and alignment,  
 1552       and reconstruction modules that process event data, so that physicists can perform  
 1553       analysis. The CMSSW event processing model is composed of one executable, called  
 1554       cmsRun, and several plug-in modules which contains all the tools (calibration, recon-

1555 struction algorithms) needed to process an event. The same executable is used for  
1556 both detector data and Monte Carlo simulations [88].

1557 **Chapter 3**

1558 **Event generation, simulation and  
1559 reconstruction**

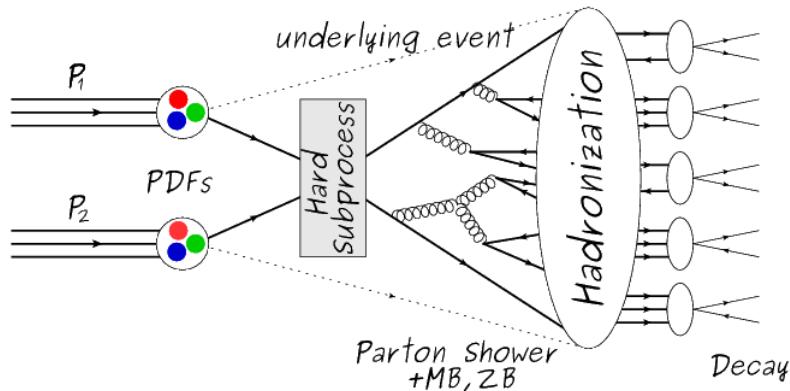
1560 The process of analyzing data recorded by the CMS experiment involves several stages  
1561 where the data are processed in order to interpret the information provided by all  
1562 the detection systems; in those stages, the particles produced after the  $pp$  collision  
1563 are identified by reconstructing their trajectories and measuring their features. In  
1564 addition, the SM provides a set of predictions that have to be compared with the  
1565 experimental results; however, in most of the cases, theoretical predictions are not  
1566 directly comparable to experimental results due to the diverse source of uncertainties  
1567 introduced by the experimental setup and theoretical approximations, among others.

1568 The strategy to face these conditions consists in using statistical methods imple-  
1569 mented in computational algorithms to produce numerical results that can be con-  
1570 trasted with the experimental results. These computational algorithms are commonly  
1571 known as Monte Carlo (MC) methods and, in the case of particle physics, they are  
1572 designed to apply the SM rules and produce predictions about the physical observ-  
1573 ables measured in the experiments. Since particle physics is governed by quantum

mechanics principles, predictions are not allowed from single events; therefore, a high number of events are *generated* and predictions are produced in the form of statistical distributions for the observables. Effects of the detector presence are included in the predictions by introducing simulations of the detector itself.

This chapter presents a description of the event generation strategy and the tools used to perform the detector simulation and physics objects reconstruction. A comprehensive review of event generators for LHC physics can be found in Reference [89] on which this chapter is based.

### 3.1 Event generation



**Figure 3.1:** Event generation process. The actual interaction is generated in the hard subprocess. The parton shower describes the evolution of the partons from the hard subprocess. Modified from Reference [90].

The event generation is intended to create events that mimic the behavior of actual events produced in collisions; they obey a sequence of steps from the particles collision hard process to the decay process into the final state. Figure 3.1 shows a schematic view of the event generation process; the fact that the full process can be treated as several independent steps is motivated by the QCD factorization theorem.

1588 Generation starts by taking into account the PDFs of the incoming particles.  
 1589 Event generators offer the option to chose from several PDF sets depending on the  
 1590 particular process under simulation<sup>1</sup>; in the following,  $pp$  collisions will be consid-  
 1591 ered. The *hard subprocess* describes the actual interaction between partons from the  
 1592 incoming protons; it is represented by the matrix element connecting the initial and  
 1593 final states of the interaction. Normally, the matrix element can be written as a  
 1594 sum over Feynman diagrams and consider interferences between terms in the sum-  
 1595 mation. During the generation of the hard subprocess, the production cross section  
 1596 is calculated.

1597 The order to which the cross section is calculated depends on the order of the Feyn-  
 1598 man diagrams involved in the calculation; therefore, radiative corrections are included  
 1599 by considering a higher order Feynman diagrams where QCD radiation dominates.  
 1600 Currently, cross sections calculated to LO do not offer a satisfactory description of the  
 1601 processes, i.e., the results are only reliable for the shape of distributions; therefore,  
 1602 NLO calculations have to be performed with the implication that the computing time  
 1603 needed is highly increased.

1604 The final parton content of the hard subprocess is subjected to the *parton shower*  
 1605 which generates the gluon radiation. Parton shower evolves the partons, i.e., glouns  
 1606 split into quark-antiquark pairs and quarks with enough energy radiate gluons giv-  
 1607 ing rise to further parton multiplication, following the DGLAP (Dokshitzer-Gribov-  
 1608 Lipatov-Altarelli-Parisi) equations. Showering continues until the energy scale is low  
 1609 enough to reach the non-perturbative limit.

1610 In the simulation of LHC processes that involve  $b$  quarks, like the single top quark  
 1611 or Higgs associated production, it is needed to consider that the  $b$  quark is heavier  
 1612 than the proton; hence, the QCD interaction description is made in two different

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<sup>1</sup> Tool in Reference [91] allows to plot different PDF sets under customizable conditions.

1613 schemes [95]

- 1614     • four-flavor (4F) scheme.  $b$  quarks appear only in the final state because they  
 1615       are heavier than the proton and therefore they can be produced only from the  
 1616       splitting of a gluon into pairs or singly in association with a  $t$  quark in high  
 1617       energy-scale interactions; furthermore, during the simulation, the  $b$ -PDFs are set  
 1618       to zero. Calculations in this scheme are more complicated due to the presence  
 1619       of the second  $b$  quark but the full kinematics is considered already at LO and  
 1620       therefore the accuracy of the description is better.
- 1621     • five-flavor (5F) scheme.  $b$  quarks are considered massless, therefore they can  
 1622       appear in both initial and final states since they can now be part of the proton;  
 1623       thus, during the simulation  $b$ -PDFs are not set to zero. In this scheme, calcula-  
 1624       tions are simpler than in the 4F scheme and possible logarithmic divergences  
 1625       are absorbed by the PDFs through the DGLAP evolution.

1626     In this thesis, the  $tHq$  events are generated using the 4F scheme in order to reduce  
 1627     uncertainties, while the  $tHW$  events are generated using the 5F scheme to eliminate  
 1628     LO interference with  $t\bar{t}H$  process [48].

1629     Partons involved in the  $pp$  collision are the focus of the simulation, however, the  
 1630     rest of the partons inside the incoming protons are also affected because the remnants  
 1631     are colored objects; also, multiple parton interactions can occur. The hadronization  
 1632     of the remnants and multiple parton interactions are known as *underlying event* and  
 1633     it has to be included in the simulation. In addition, multiple  $pp$  collisions in the same  
 1634     bunch crossing (pile-up mentioned in 2.2) occurs, actually in two forms

- 1635     • *in-time PU* which refers to multiple  $pp$  collision in the bunch crossing but that  
 1636       are not considered as primary vertices.

1637       • *Out-of-time PU* which refers to overlapping  $pp$  collisions from consecutive bunch  
 1638       crossings; this can occur due to the time-delays in the detection systems where  
 1639       information from one bunch crossing is assigned to the next or previous one.

1640       While the underlying event effects are included in generation using generator-  
 1641       specific tools, PU effects are added to the generation by overlaying Minimum-bias (MB)  
 1642       and Zero-bias (ZB) events to the generated events. MB events are inelastic events  
 1643       selected by using a loose trigger with as little bias as possible, therefore accepting a  
 1644       large fraction of the overall inelastic event; ZB events correspond to random events  
 1645       recorded by the detector when collisions are likely. MB models in-time PU and ZB  
 1646       models out-of-time PU.

1647       The next step in the generation process is called *hadronization*. Since particles  
 1648       with a net color charge are not allowed to exits isolated, they have to recombine  
 1649       to form bound states. This is precisely the process by which the partons resulting  
 1650       from the parton shower arrange themselves as color singlets to form hadrons. At  
 1651       this step, the energy-scale is low and the strong coupling constant is large, therefore  
 1652       hadronization process is non-perturbative and the evolution of the partons is described  
 1653       using phenomenological models. Most of the baryons and mesons produced in the  
 1654       hadronization are unstable and hence they will decay in the detector.

1655       The last step in the generation process corresponds to the decay of the unstable  
 1656       particles generated during hadronization; it is also simulated in the hadronization  
 1657       step, based on the known branching ratios.

## 1658       **3.2 Monte Carlo Event Generators.**

1659       The event generation described in the previous section has been implemented in  
 1660       several software packages for which a brief description is given.

- 1661     • **PYTHIA 8.** It is a program designed to perform the generation of high energy  
 1662        physics events which describes the collisions between particles such as electrons  
 1663        and protons. Several theories and models are implemented in it, in order to  
 1664        describe physical aspects like hard and soft interaction, parton distributions,  
 1665        initial and final-state parton showers, multiple parton interactions, beam rem-  
 1666        nants, hadronization<sup>2</sup> and particle decay. Thanks to extensive testing, several  
 1667        optimized parametrizations, known as *tunings*, have been defined in order to  
 1668        improve the description of actual collisions to a high degree of precision; for  
 1669        analysis at  $\sqrt{s} = 13$  TeV, the underline event CUETP8M1 tune is employed [97].  
 1670        The calculation of the matrix element is performed at LO which is not enough  
 1671        for the current required level of precision; therefore, pythia is often used for  
 1672        parton shower, hadronization and decays, while other event generators are used  
 1673        to generate the matrix element at NLO.
- 1674     • **MadGraph5\_aMC@NLO.** MadGraph is a matrix element generator which  
 1675        calculates the amplitudes for all contributing Feynman diagrams of a given  
 1676        process but does not provide a parton shower while MC@NLO incorporates  
 1677        NLO QCD matrix elements consistently into a parton shower framework; thus,  
 1678        MadGraph5\_aMC@NLO, as a merger of the two event generators MadGraph5  
 1679        and aMC@NLO, is an event generator capable to calculate tree-level and NLO  
 1680        cross sections and perform the matching of those with the parton shower. It is  
 1681        one of the most frequently used matrix element generators; however, it has the  
 1682        particular feature of the presence of negative event weights which reduce the  
 1683        number of events used to reproduce the properties of the objects generated [98].
- 1684     • **POWHEG.** It is an NLO matrix element generator where the hardest emis-

---

<sup>2</sup> based in the Lund string model [96]

1685 sion of color charged particles is generated in such a way that the negative event  
 1686 weights issue of MadGraph5\_aMC@NLO is overcome; however, the method re-  
 1687 quires an interface with  $p_T$ -ordered parton shower or a parton shower generator  
 1688 where this highest emission can be vetoed in order to avoid double counting of  
 1689 this highest-energetic emission. PYTHIA is a commonly matched to POWHEG  
 1690 event generator [100].

1691 Events resulting from the whole generation process are known as MC events.

### 1692 3.3 CMS detector simulation.

1693 After generation, MC events contain the physics of the collisions but they are not  
 1694 ready to be compared to the events recorded by the experiment since these recorded  
 1695 events correspond to the response of the detection systems to the interaction with  
 1696 the particles traversing them. The simulation of the CMS detector has to be applied  
 1697 on top of the event generation; it is simulated with a MC toolkit for the simulation  
 1698 of particles passing through matter called Geant4 which is also able to simulate the  
 1699 electronic signals that would be measured by all detectors inside CMS.

1700 The simulation takes the generated particles contained in the MC events as input,  
 1701 makes them pass through the simulated geometry, and models physics processes that  
 1702 particles experience during their passage through matter. The full set of results from  
 1703 particle-matter interactions corresponds to the simulated hit which contains informa-  
 1704 tion about the energy loss, momentum and position. Particles of the input event are  
 1705 called *primary*, while the particles originating from GEANT4-modeled interactions of  
 1706 a primary particle with matter are called a *secondary*. Simulated hits are the input  
 1707 of subsequent modules that emulate the response of the detector readout system and

1708 triggers. The output from the emulated detection systems and triggers is known as  
 1709 digitization [101, 102].

1710 The modeling of the CMS detector corresponds to the accurate modeling of the  
 1711 interaction among particles, the detector material, and the magnetic field. This  
 1712 simulation procedure includes the following standard steps

1713 • Modeling of the Interaction Region.

1714 • Modeling of the particle passage through the hierarchy of volumes that compose  
 1715 CMS detector and of the accompanying physics processes.

1716 • Modeling of the effect of multiple interactions per beam crossing and/or the  
 1717 effect of events overlay ( Pile-Up simulation).

1718 • Modeling of the detector's electronics response, signal shape, noise, calibration  
 1719 constants (digitization).

1720 In addition to the full simulation, i.e., a detailed detector simulation, a faster  
 1721 simulation (FastSim) have been developed, that may be used where much larger  
 1722 statistics are required. In FastSim, detector material effects are parametrized and  
 1723 included in the hits; those hits are used as input of the same higher-level algorithms<sup>3</sup>  
 1724 used to analyze the recorded events. In this way, comparisons between fast and full  
 1725 simulations can be performed [104].

1726 After the full detector simulation, the output events can be directly compared  
 1727 to events actually recorded in the CMS detector. The collection of MC events that  
 1728 reproduces the expected physics for a given process is known as MC sample.

---

<sup>3</sup> track fitting, calorimeter clustering, b tagging, electron identification, jet reconstruction and calibration, trigger algorithms which will be considered in the next sections

1729 **3.4 Event reconstruction.**

1730 The CMS experiment use the *particle-flow event reconstruction algorithm (PF)* to do  
1731 the reconstruction of particles produced in  $pp$  collisions. Next sections will present  
1732 a basic description of the *Elements* used by PF (tracker tracks, energy clusters, and  
1733 muon tracks), based in the References [105, 106] where more detailed descriptions can  
1734 be found.

1735 **3.4.1 Particle-Flow Algorithm.**

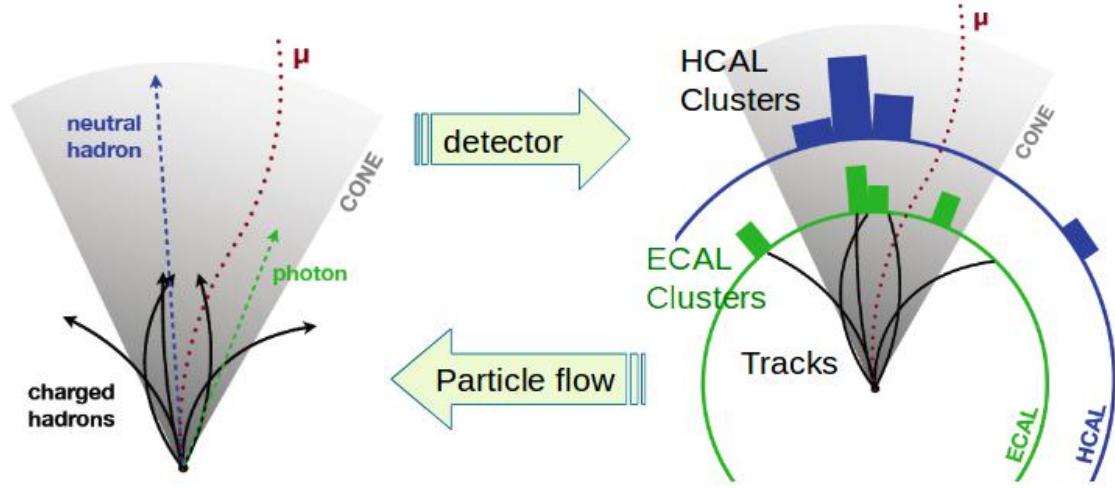
1736 Each of the several sub detection systems of the CMS detector is dedicated to identify  
1737 an specific type of particles, i.e., photons and electrons are absorbed by the ECAL  
1738 and their reconstruction is based on ECAL information; hadrons are reconstructed  
1739 from clusters in the HCAL while muons are reconstructed from hits in the muon  
1740 chambers. PF is designed to correlate signals from all the detector layers (tracks and  
1741 energy clusters) in order to reconstruct and identify each final state particle and its  
1742 properties as sketched in Figure 3.2.

1743 For instance, a charged hadron is identified by a geometrical connection, known  
1744 as *link*, between one or more calorimeter clusters and a track in the tracker, provided  
1745 there are no hits in the muon system; combining several measurements allows a better  
1746 determination of the energy and charge sign of the charged hadron.

1747 **Charged-particle track reconstruction.**

1748 The strategy used by PF in order to reconstruct tracks is called *Iterative Tracking*  
1749 which occurs in four steps

- 1750 • Seed generation where initial track candidates are found by looking for a combi-  
1751 nation of hits in the pixel detector, strip tracker, and muon chambers. In total



**Figure 3.2:** Particle flow algorithm. Information from the several CMS detection systems is provided as input to the algorithm which then combines it to identify and reconstruct all the particles in the final state and their properties. Reconstruction of simulated events is also performed by providing information from MC samples, detector and trigger simulation [107].

1752 ten iterations are performed, each one with a different seeding requirement.  
 1753 Seeds are used to estimate the trajectory parameters and uncertainties at the  
 1754 time of the full track reconstruction. Seeds are also considered track candidates.

- 1755 • Track finding using a tracking software known as Combinatorial Track Finder  
 1756 (CTF) [108]. The seed trajectories are extrapolated along the expected flight  
 1757 path of a charged particle, in agreement to the trajectory parameters obtained  
 1758 in the first step, in an attempt to find additional hits that can be assigned to  
 1759 the track candidates.

- 1760 • Track-fitting where the found tracks are passed as input to a module which  
 1761 provides the best estimate of the parameters of each trajectory.

- 1762 • Track selection where track candidates are submitted to a selection which dis-  
 1763 cards those that fail a set of defined quality criteria.

1764 Iterations differ in the seeding configuration and the final track selection as elab-

1765 orated in References [105, 106]. In the first iteration, high  $p_T$  tracks and tracks pro-  
 1766 duced near to the interaction region are identified and those hits are masked thereby  
 1767 reducing the combinatorial complexity. Next, iterations search for more complicated  
 1768 tracks, like low  $p_T$  tracks and tracks from b hadron decays, which tend to be displaced  
 1769 from the interaction region.

1770 **Vertex reconstruction.**

1771 During the track reconstruction, an extrapolation toward to the calorimeters is per-  
 1772 formed in order to match energy deposits; that extrapolation is performed also toward  
 1773 the beamline in order to find the origin of the track known as *vertex*. The vertex re-  
 1774 construction is performed by selecting from the available reconstructed tracks, those  
 1775 that are consistent with being originated in the interaction region where  $pp$  collisions  
 1776 are produced. The selection involves a requirement on the number of tracker (pixel  
 1777 and strip) hits and the goodness of the track fit.

1778 Selected tracks are clustered using a *deterministic annealing algorithm* (DA)<sup>4</sup>. A  
 1779 set of candidate vertices and their associated tracks, resulting from the DA, are then  
 1780 fitted with an *adaptive vertex fitter* (AVF) to produce the best estimate of the vertices  
 1781 locations.

1782 The  $p_T$  of the tracks associated to a reconstructed vertex is added, squared and  
 1783 used to organize the vertices; the vertex with the highest squared sum is designated  
 1784 as the *primary vertex* (PV) while the rest are designated as PU vertices.

1785 **Calorimeter clustering.**

1786 After traversing the CMS tracker system, electrons, photons and hadrons deposit their  
 1787 energy in the ECAL and HCAL cells. The PF clustering algorithm aims to provide

---

<sup>4</sup> DA algorithm and AVF are described in detail in References [110, 111]

1788 a high detection efficiency even for low-energy particles and an efficient distinction  
 1789 between close energy deposits. The clustering runs independently in the ECAL barrel  
 1790 and endcaps, HCAL barrel and endcaps, and the two preshower layers, following two  
 1791 steps

- 1792     • cells with an energy larger than a given seed threshold and larger than the energy  
     1793        of the neighboring cells are identified as cluster seeds. The neighbor cells are  
     1794        those that either share a side with the cluster seed candidate, or the eight closest  
     1795        cells including cells that only share a corner with the seed candidate.
- 1796     • cells with at least a corner in common with a cell already in the cluster seed  
     1797        and with an energy above a cell threshold are grouped into topological clusters.

1798 Clusters formed in this way are known as *particle-flow clusters*. With this cluster-  
 1799 ing strategy, it is possible to detect and measure the energy and direction of photons  
 1800 and neutral hadrons as well as differentiate these neutral particles from the charged  
 1801 hadron energy deposits. In cases involving charged hadrons for which the track pa-  
 1802 rameters are not determined accurately, for instance, low-quality and high- $p_T$  tracks,  
 1803 clustering helps in the energy measurements.

#### 1804 **Electron track reconstruction.**

1805 Although the charged-particle track reconstruction described above works for elec-  
 1806 trons, they lose a significant fraction of their energy via bremsstrahlung photon radi-  
 1807 ation before reaching the ECAL; thus, the reconstruction performance depends on the  
 1808 ability to measure also the radiated energy. The reconstruction strategy, in this case,  
 1809 requires information from the tracking system and from the ECAL. Bremsstrahlung  
 1810 photons are emitted at similar  $\eta$  values to that of the electron but at different values  
 1811 of  $\phi$ ; therefore, the radiated energy can be recovered by grouping ECAL clusters in a

1812    $\eta$  window over a range of  $\phi$  around the electron direction. The group is called ECAL  
 1813   supercluster.

1814       Electron candidates from the track-seeding and ECAL super clustering are merged  
 1815   into a single collection which is submitted to a full electron tracking fit with a  
 1816   Gaussian-sum filter (GSF) [109]. The electron track and its associated ECAL su-  
 1817   percluster form a *particle-flow electron*.

1818   **Muon track reconstruction.**

1819   Given that the CMS detector is equipped with a muon spectrometer capable to iden-  
 1820   tify and measure the momentum of the muons traversing it, the muon reconstruction  
 1821   is not specific to PF; therefore, three different muon types are defined

- 1822       • *Standalone muon.* A clustering on the DTs or CSCs hits is performed to form  
   1823       track segments; those segments are used as seeds for the reconstruction in the  
   1824       muon spectrometer. All DTs, CSCs, and RPCs hits along the muon trajectory  
   1825       are combined and fitted to form the full track. The fitting output is called a  
   1826       *standalone-muon track*.
- 1827       • *Tracker muon.* Each track in the inner tracker with  $p_T$  larger than 0.5 GeV and  
   1828       a total momentum  $p$  larger than 2.5 GeV is extrapolated to the muon system.  
   1829       A *tracker muon track* corresponds to a extrapolated track that matches at least  
   1830       one muon segment.
- 1831       • *Global muon.* When tracks in the inner tracker (inner tracks) and standalone-  
   1832       muon tracks are matched and turn out being compatibles, their hits are com-  
   1833       bined and fitted to form a *global-muon track*.

1834        Global muons sharing the same inner track with tracker muons are merged into  
 1835      a single candidate. PF muon identification uses the muon energy deposits in ECAL,  
 1836      HCAL, and HO associated with the muon track to improve the muon identification.

1837 **Particle identification and reconstruction.**

1838      PF elements are connected by a linker algorithm that tests the connection between any  
 1839      pair of elements; if they are found to be linked, a geometrical distance that quantifies  
 1840      the quality of the link is assigned. Two elements may be linked indirectly through  
 1841      common elements. Linked elements form *PF blocks* and each PF block may contain  
 1842      elements originating in one or more particles. Links can be established between  
 1843      tracks, between calorimeter clusters, and between tracks and calorimeter clusters.  
 1844      The identification and reconstruction start with a PF block and proceed as follows

1845        • Muons. An *isolated global muon* is identified by evaluating the presence of  
 1846      inner track and energy deposits close to the global muon track in the  $(\eta, \phi)$   
 1847      plane, i.e., in a particular point of the global muon track, inner tracks and  
 1848      energy deposits are sought within a radius of  $\Delta R = 0.3$  (see eqn. 2.7) from the  
 1849      muon track; if they exist and the  $p_T$  of the found track added to the  $E_T$  of the  
 1850      found energy deposit does not exceed 10% of the muon  $p_T$  then the global muon  
 1851      is an isolated global muon. This isolation condition is stringent enough to reject  
 1852      hadrons misidentified as muons.

1853        *Non-isolated global muons* are identified using additional selection requirements  
 1854      on the number of track segments in the muon system and energy deposits along  
 1855      the muon track. Muons inside jets are identified with more stringent criteria  
 1856      in isolation and momentum as described in Reference [112]. The PF elements  
 1857      associated with an identified muon are masked from the PF block.

- 1858     ● Electrons are identified and reconstructed as described above plus some addi-  
 1859         tional requirements on fourteen variables like the amount of energy radiated,  
 1860         the distance between the extrapolated track position at the ECAL and the po-  
 1861         sition of the associated ECAL supercluster, among others, which are combined  
 1862         in an specialized multivariate analysis strategy that improves the electron iden-  
 1863         tification. Tracks and clusters used to identify and reconstruct electrons are  
 1864         masked in the PF block.
- 1865     ● Isolated photons are identified from ECAL superclusters with  $E_T$  larger than 10  
 1866         GeV, for which the energy deposited at a distance of 0.15, from the supercluster  
 1867         position on the  $(\eta, \phi)$  plane, does not exceed 10% of the supercluster energy;  
 1868         note that this is an isolation requirement. In addition, there must not be links  
 1869         to tracks. Clusters involved in the identification and reconstruction are masked  
 1870         in the PF block.
- 1871     ● Bremsstrahlung photons and prompt photons tend to convert to electron-positron  
 1872         pairs inside the tracker, therefore, a dedicated finder algorithm is used to link  
 1873         tracks that seem to originate from a photon conversion; in case those two tracks  
 1874         are compatible with the direction of a bremsstrahlung photon, they are also  
 1875         linked to the original electron track. Photon conversion tracks are also masked  
 1876         in the PF block.
- 1877     ● The remaining elements in the PF block are used to identify hadrons. In the  
 1878         region  $|\eta| \leq 2.5$ , neutral hadrons are identified with HCAL clusters not linked  
 1879         to any track while photons from neutral pion decays are identified with ECAL  
 1880         clusters without links to tracks. In the region  $|\eta| > 2.5$  ECAL clusters linked to  
 1881         HCAL clusters are identified with a charged or neutral hadron shower; ECAL  
 1882         clusters with no links are identified with photons. HCAL clusters not used yet,

1883        are linked to one or more unlinked tracks and to an unlinked ECAL in order to  
 1884        reconstruct charged-hadrons or a combination of photons and neutral hadrons  
 1885        according to certain conditions on the calibrated calorimetric energy.

- 1886        • Charged-particle tracks may be liked together when they converge to a *sec-*  
 1887        *ondary vertex (SV)* displaced from the IP where the PV and PU vertices are  
 1888        reconstructed; at least three tracks are needed in that case, of which at most  
 1889        one has to be an incoming track with hits in tracker region between a PV and  
 1890        the SV.

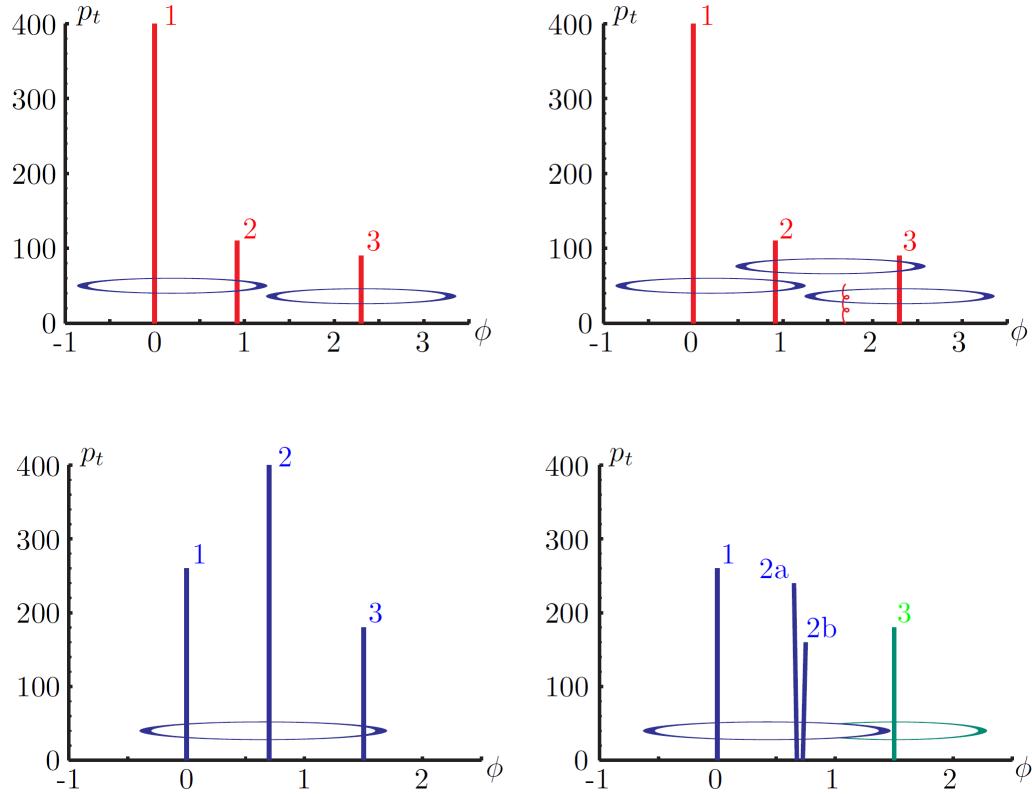
1891        The linker algorithm, as well as the whole PF algorithm, has been validated and  
 1892        commissioned; results from that validation are presented in the Reference [105].

1893 **Jet reconstruction.**

1894        Quarks and gluons may be produced in the  $pp$  collisions, therefore, their hadronization  
 1895        will be seen in the detector as a shower of hadrons and their decay products in the  
 1896        form of a *jet*. Two classes of clustering algorithms have been developed based in  
 1897        their jet definition [113]:

- 1898        • Iterative cone algorithms (IC). Jets are defined in terms of circles of fixed radius  
 1899         $R$  in the  $\eta\text{-}\phi$  plane, known as *stable cones*, for which the sum of the momenta  
 1900        of all the particles within the cone points in the same direction as the center  
 1901        of the circle. The seed of the iteration is the hardest non-isolated particle in  
 1902        the event, then, the resulting momentum direction is assigned as the new cone  
 1903        direction and a new iteration starts; iteration process stops when the cone if  
 1904        found to be stable.

- 1905     • Sequential recombination algorithms. The distance between non-isolated par-  
 1906        ticles is calculated; if that distance is below a threshold, these particles are  
 1907        recombined into a new object. The sequence is repeated until the separation  
 1908        between the recombined object and any other particle is above certain thresh-  
 1909        old; the recombined object is called a jet and the algorithm starts again with  
 1910        the remaining particles.



**Figure 3.3:** Stable cones identification using IC algorithms [113].

- 1911        Two conditions are of particular importance for the clustering algorithms, *infrared*  
 1912        and *collinear (IRC) safety*. In order to explain the concept of infrared (IR) safety,  
 1913        consider an event with three hard particles as shown in the top left side of Figure 3.3,  
 1914        two stable cones are found and then two jets are identified; if a soft gluon is added, as  
 1915        shown in the top right side of Figure 3.3, three stable cones are found and the three

1916 hard particles are now clustered into a single jet. If the addition of soft particles  
 1917 change the outcome of the clustering, then it is said that the algorithm is IR unsafe.  
 1918 Soft radiation is highly likely in perturbative QCD, which dominates the physics of  
 1919 the jets, and then IR unsafe effect leads to divergences [113].

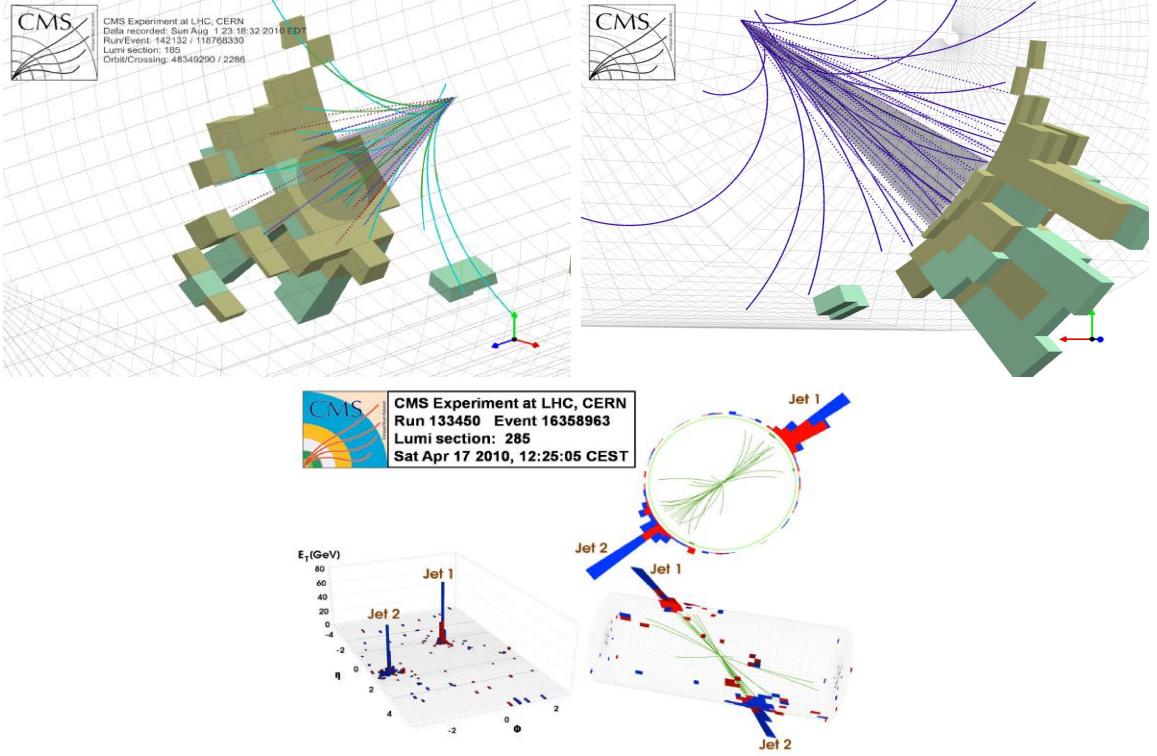
1920 The concept of collinear safety can also be explained considering a three hard  
 1921 particles event, as shown in the bottom left side of Figure 3.3, where one stable cone  
 1922 containing all three particles is found and one jet is identified; if the hardest particle  
 1923 is split into two collinear particles (2a and 2b) in the bottom right side of Figure 3.3,  
 1924 then the clustering results in a different jet identification and the algorithm is said  
 1925 to be collinear unsafe. The collinear unsafe effect leads to divergences in jet cross  
 1926 section calculations [114].

1927 It has been determined that IC algorithms are IRC unsafe, and therefore, they  
 1928 have to be replaced by algorithms that not only provide the finite perturbative results  
 1929 from theoretical computations, but also that are not highly dependent on underlying  
 1930 event and pileup effects which leads to significant corrections [113].

1931 The sequential recombination algorithms arise as the IRC safe alternative used by  
 1932 the CMS experiment; in particular the anti- $k_t$  algorithm which is a generalization of  
 1933 the previously existing  $k_t$  [115] and Cambridge/Aachen [116] jet clustering algorithms.

1934 The anti- $k_t$  algorithm is used to perform the jet reconstruction by clustering those  
 1935 PF particles within a cone (see Figure 3.4); previously, isolated electrons, isolated  
 1936 muons, and charged particles associated with other interaction vertices are excluded  
 1937 from the clustering.

1938 The anti- $k_t$  algorithm proceeds in a sequential recombination of PF particles; the  
 1939 distance between particles  $i$  and  $j$  ( $d_{ij}$ ) and the distance between particles and the  
 1940 beam are defined as



**Figure 3.4:** Jet reconstruction performed by the anti- $k_t$  algorithm. Top: Two different views of a CMS recorded event are presented. Continuous lines correspond to tracks left by charged particles in the tracker while dotted lines are the imaginary paths followed by neutral particles. The green cubes represent the ECAL cells while the blue ones represent the HCAL cells; in both cases, the height of the cube represent the amount of energy deposited in the cells [117]. Bottom: Reconstruction of a recorded event with two jets [118].

$$d_{ij} = \min\left(\frac{1}{k_{ti}^2}, \frac{1}{k_{tj}^2}\right) \frac{\Delta_{ij}^2}{R^2}$$

$$d_{iB} = \frac{1}{k_{ti}^2} \quad (3.1)$$

1941 where  $\Delta_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$ ,  $k_{ti}$ ,  $y_i$  and  $\phi_i$  are the transverse momentum, ra-  
 1942 pidity and azimuth of particle  $i$  respectively and  $R$  is the called jet radius. For all  
 1943 the remaining PF particles, after removing the isolated ones,  $d_{ij}$  and  $d_{iB}$  are calcu-

1944 lated<sup>5</sup> and the smallest is identified; if it is a  $d_{ij}$ , particles  $i$  and  $j$  are replaced with  
 1945 a new object whose momentum is the vectorial sum of the combined particles. If the  
 1946 smallest distance is a  $d_{iB}$  the clustering process ends, the object  $i$  (which at this stage  
 1947 should be a combination of several PF particles) is declared as a *Particle-flow-jet* (PF  
 1948 jet) and all the associated PF particles are removed from the detector. The clustering  
 1949 process is repeated until no PF particles remain.  $R$  is a free parameter that can be  
 1950 adjusted according to the specific analysis conditions; usually, two values are used,  
 1951  $R=0.4$  and  $R=0.5$ , giving the name to the so-called AK4-jet and AK5-jet respectively.

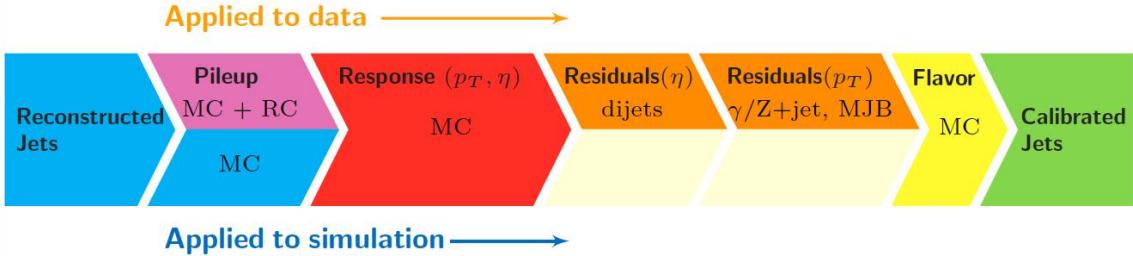
1952 An advantage of the anti- $k_t$  algorithm over other clustering algorithms is the reg-  
 1953 ularity of the boundaries of the resulting jets. For all known IRC safe algorithms,  
 1954 soft radiation can introduce irregularities in the boundaries of the final jets; however,  
 1955 anti- $k_t$  algorithm is soft-resilient, meaning that jets shape is not affected by soft radi-  
 1956 ation, which is a valuable property considering that knowing the typical shape of jets  
 1957 makes experimental calibration of jets more simple. In addition, that soft-resilience  
 1958 is expected to simplify certain theoretical calculations and reduce the momentum-  
 1959 resolution loss caused by underlying-event (UE) and pileup contamination [114].

1960 The effect of the UE and pileup contamination over a jet identification, can be  
 1961 seen as if soft events are added to the jet; for instance, if a soft event representing UE  
 1962 or pileup is added to an event for which a set of jets  $J$  have been identified, and the  
 1963 clustering is rerun on that new extended event, the outcome will be different in two  
 1964 aspects: jets will contain some additional soft energy and the distribution of particles  
 1965 in jets may have change; that effect is called *back-reaction*. The back-reaction effect in  
 1966 the anti- $k_t$  algorithm is suppressed not by the amount of momentum added to the jet  
 1967 but by the jet transverse momentum  $p_{T,J}$ , which means that this strong suppression  
 1968 leads to a smaller correction due to EU and pileup effect [114].

---

<sup>5</sup> Notice that this is a combinatorial calculation.

1969 **Jet energy Corrections**



**Figure 3.5:** Jet energy correction diagram. Correction levels are applied sequentially in the indicated fixed order [120].

1970 Even though jets can be reconstructed efficiently, there are some effects that are  
 1971 not included in the reconstruction and that lead to discrepancies between the re-  
 1972 constructed results and the predicted results; in order to overcome these discrep-  
 1973 ancies, a factorized model has been designed in the form of jet energy corrections  
 1974 (JEC) [119, 120] applied sequentially as shown in the diagram of Figure 3.5.

1975 At each level, the jet four-momentum is multiplied by a scaling factor based on  
 1976 jet properties, i.e.,  $\eta$ , flavor, etc.

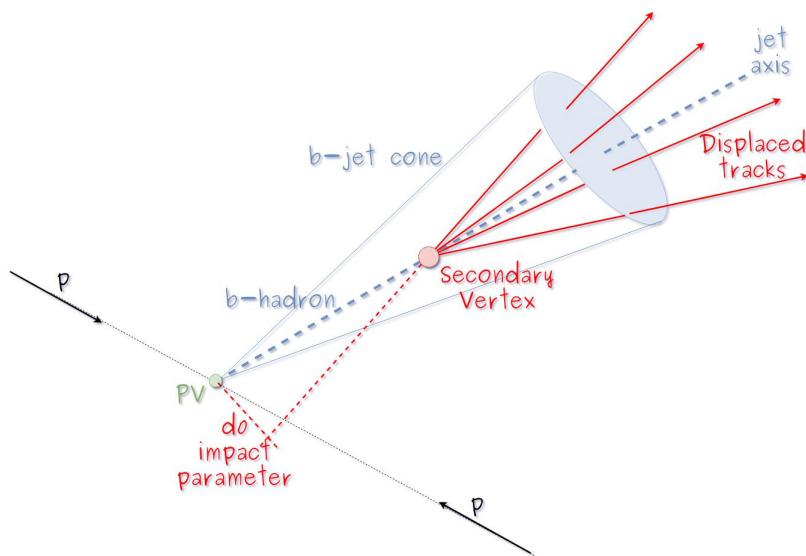
- 1977 • Level 1 correction removes the energy coming from pile-up. The scale factor is  
 1978 determined using a MC sample of QCD dijet (2 jets) events with and without  
 1979 pileup overlay; it is parametrized in terms of the offset energy density  $\rho$ , jet  
 1980 area  $A$ , jet  $\eta$  and jet  $p_T$ . Different corrections are applied to data and MC due  
 1981 to the detector simulation.
- 1982 • MC-truth correction accounts for differences between the reconstructed jet en-  
 1983 ergy and the MC particle-level energy. The correction is determined on a QCD  
 1984 dijet MC sample and is parametrized in terms of the jet  $p_T$  and  $\eta$ .
- 1985 • Residuals correct remaining small differences within jet response in data and  
 1986 MC. The Residuals  $\eta$ -dependent correction compares jets of similar  $p_T$  in the

1987 barrel reference region. The Residuals  $p_T$ -dependent correct the jet absolute  
 1988 scale (JES vs  $p_T$ ).

- 1989 • Jet-flavor corrections are derived in the same way as MC-truth corrections but  
 1990 using QCD pure flavor samples.

1991 ***b*-tagging of jets.**

1992 A particular feature of the hadrons containing bottom quarks (*b*-hadrons) is that  
 1993 their lifetime is long enough to travel some distance before decaying, but it is not as  
 1994 long as those of light quark hadrons; therefore, when looking at the hadrons produced  
 1995 in  $pp$  collisions, *b*-hadrons decay typically inside the tracker rather than reaching the  
 1996 calorimeters as some light-hadrons do. As a result, a *b*-hadron decay gives rise to a  
 1997 displaced vertex (secondary vertex) with respect to the primary vertex as shown in  
 1998 Figure 3.6; the SV displacement is in the order of a few millimeters. A jet resulting  
 1999 from the decay of a *b*-hadron is called *b* jet; other jets are called light jets.



**Figure 3.6:** Secondary vertex in a *b*-hadron decay.

2000 Several methods to identify *b*-jets (*b*-tagging) have been developed; the method

used in this thesis is known as *Combined Secondary Vertex* algorithm in its second version (CSVv2) [121]. By using information of the impact parameter, the reconstructed secondary vertices, and the jet kinematics as input in a multivariate analysis that combines the discrimination power of each variable in one global discriminator variable, three working points (references): loose, medium and tight, are defined which quantify the probabilities of mistag jets from light quarks as jets from  $b$  quarks; 10, 1 and 0.1 % respectively. Although the mistagging probability decreases with the working point strength, the efficiency to correctly tag  $b$ -jets also decreases as 83, 69 and 49 % for the respective working point; therefore, a balance needs to be achieved according to the specific requirements of the analysis.

### Missing transverse energy.

The fact that proton bunches carry momentum along the  $z$ -axis implies that for each event it is expected that the momentum in the transverse plane is balanced. Imbalances are quantified by the missing transverse energy (MET) and are attributed to several sources including particles escaping undetected through the beam pipe, neutrinos produced in weak interactions processes which do not interact with the detector and thus escaping without leaving a sign, or even undiscovered particles predicted by models beyond the SM.

The PF algorithm assigns the negative sum of the momenta of all reconstructed PF particles to the *particle-flow MET* according to

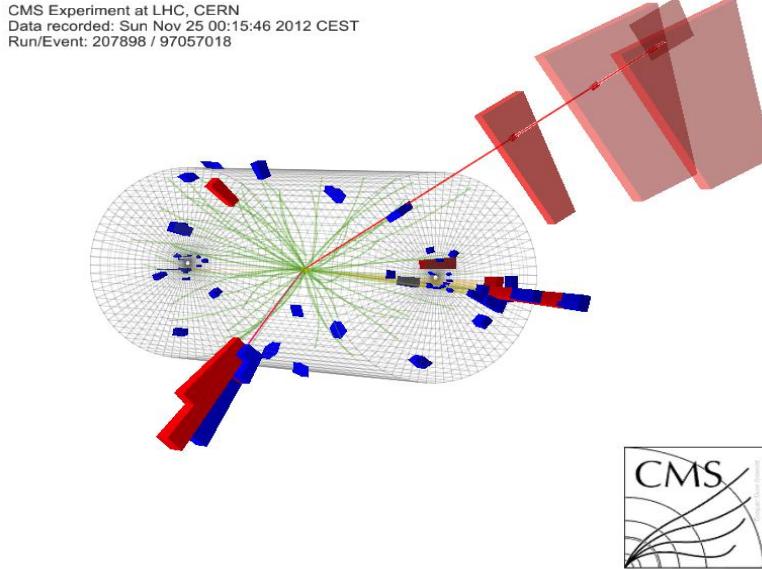
$$\vec{E}_T = - \sum_i \vec{p}_{T,i} \quad (3.2)$$

JEC are propagated to the calculation of the  $\vec{E}_T$  as described in the Reference [122].

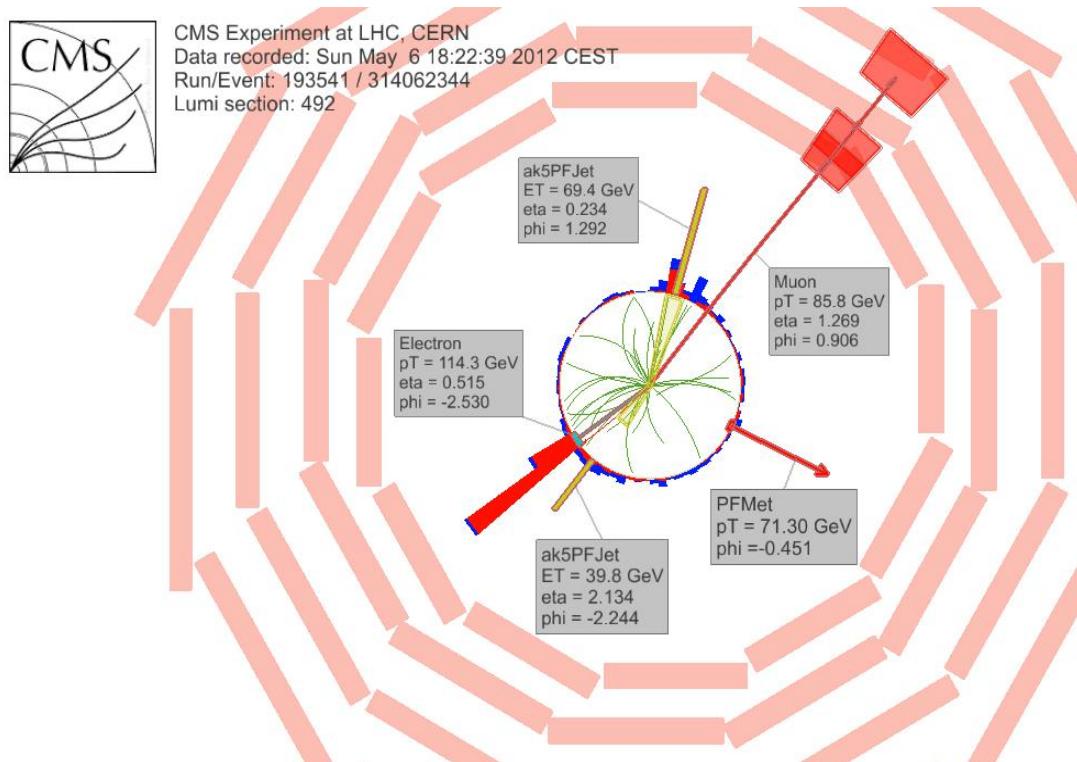
### 2022 3.4.2 Event reconstruction examples

2023 Figures 3.7-3.9 show the results of the reconstruction performed on 3 recorded events.

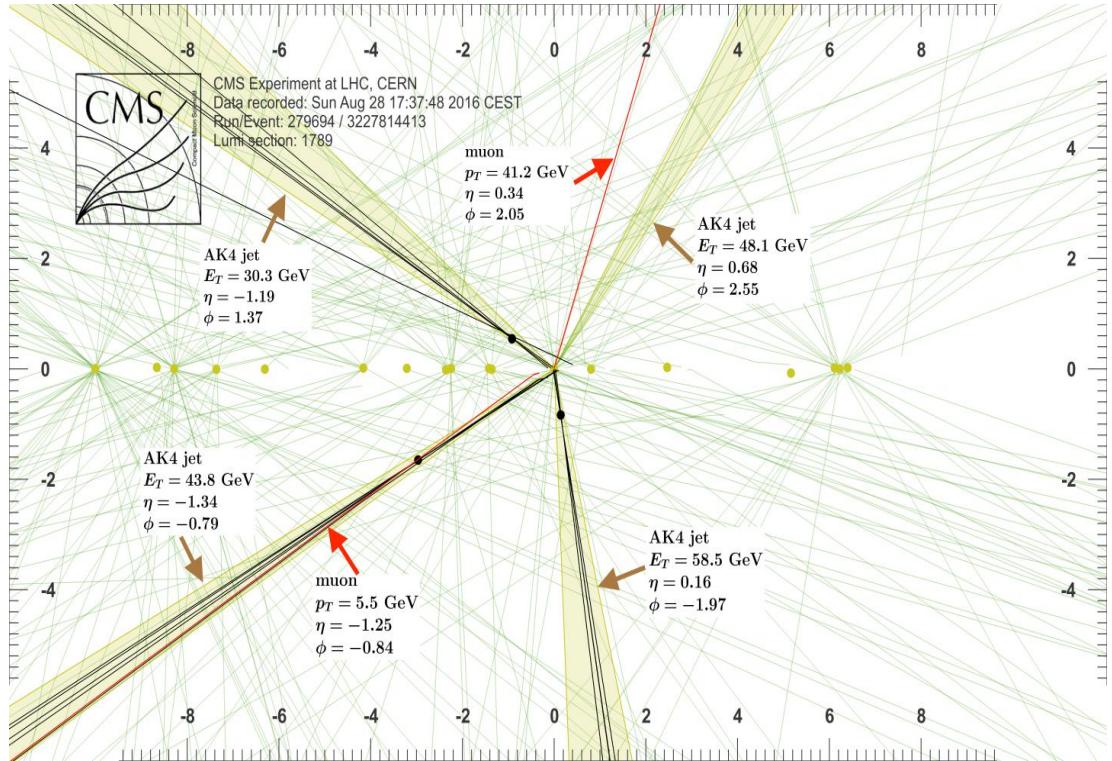
2024 Descriptions are taken directly from the source.



**Figure 3.7:** HIG-13-004 Event 1 reconstruction results; “HIG-13-004 Event 1: Event recorded with the CMS detector in 2012 at a proton-proton center-of-mass energy of 8 TeV. The event shows characteristics expected from the decay of the SM Higgs boson to a pair of  $\tau$  leptons. Such an event is characterized by the production of two forward-going jets, seen here in opposite endcaps. One of the  $\tau$  decays to a muon (red lines on the right) and neutrinos, while the other  $\tau$  decays into a charged hadron and a neutrino.” [123].



**Figure 3.8:**  $e\mu$  event reconstruction results; “An  $e\mu$  event candidate selected in 8 TeV data, as seen from the direction of the proton beams. The kinematics of the main objects used in the event selection are highlighted: two isolated leptons and two particle-flow jets. The reconstructed missing transverse energy is also displayed for reference” [124].



**Figure 3.9:** Recorded event reconstruction results;“Recorded event ( $\rho$ - $z$  projection) with three jets with  $p_T > 30$  GeV with one displaced muon track in 2016 data collected at 13 TeV. Each of the three jets has a displaced reconstructed vertex. The jet with  $p_T(j) = 43.8$  GeV,  $\eta(j) = -1.34$ ,  $\phi(j) = -0.79$  contains muon with  $p_T(\mu) = 5.5$  GeV,  $\eta(\mu) = -1.25$ ,  $\phi(\mu) = -0.84$ . Event contains reconstructed isolated muon with  $p_T(\mu) = 41.2$  GeV,  $\eta(\mu) = 0.34$ ,  $\phi(\mu) = 2.05$  and MET with  $p_T = 72.5$  GeV,  $\phi = -0.32$ . Jet candidates for a  $b$ -jet from top quark leptonic and hadronic decays are tagged by CSVv2T algorithm. One of the other two jets is tagged by CharmT algorithm. Tracks with  $p_T > 0.5$  GeV are shown. The number of reconstructed primary vertices is 18. Reconstructed  $m_T(W)$  is 101.8 GeV. Beam spot position correction is applied. Reconstructed primary vertices are shown in yellow color, while reconstructed displaced vertices and associated tracks are presented in black color. Dimensions are given in cm” [125].

2025 **Chapter 5**

2026 **Statistical methods**

2027 In the course of analyzing the data sets provided by the CMS experiment and used in  
2028 this thesis, several statistical tools have been employed; in this chapter, a description  
2029 of these tools will be presented, starting with the general statement of the multivariate  
2030 analysis methods, followed by the particularities of the Boosted Decision Trees (BDT)  
2031 method and its application to the classification problem. Statistical inference methods  
2032 used will also be presented. This chapter is based mainly on References [126–128].

2033 **5.1 Multivariate analysis**

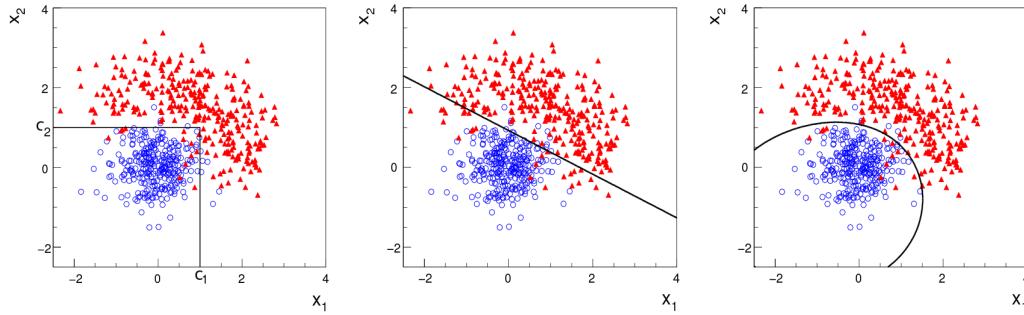
2034 Multivariate data analysis (MVA) makes use of the statistical techniques developed to  
2035 analyze more than one variable at once, taking into account all the correlations among  
2036 variables. MVA is employed in a variety of fields like consumer and market research,  
2037 quality control and process optimization. Using MVA it is possible to identify the  
2038 dominant patterns in a data sample, like groups, outliers and trends, and determine  
2039 to which group a set of values belong; in the particle physics context, MVA methods  
2040 are used to perform the selection of certain type of events from a large data set.

2041 Processes with small cross section, such as the  $tHq$  process ( $\sigma_{SM}(\sqrt{s} = 13\text{TeV}) =$   
 2042  $70.96 \text{ fb}$ ), are hard to detect in the presence of the processes with larger cross sections,  
 2043  $\sigma_{SM}^{t\bar{t}}(\sqrt{s} = 13\text{TeV}) = 823.44 \text{ fb}$  for instance; therefore, only a small fraction of the data  
 2044 contains events of interest (signal), the major part is signal-like events, which mimic  
 2045 signal characteristics but belong to different processes, so they are a background to  
 2046 the process of interest. This implies that it is not possible to say with certainty  
 2047 that a given event is a signal or a background and statistical methods should be  
 2048 involved. In that sense, the challenge can be formulated as one where a set of events  
 2049 have to be classified according to certain special features; these features correspond  
 2050 to the measurements of several parameters like energy or momentum, organized in a  
 2051 set of *input variables*. The measurements for each event can be written in a vector  
 2052  $\mathbf{x} = (x_1, \dots, x_n)$  for which

- 2053 •  $f(\mathbf{x}|s)$  is the probability density (*likelihood function*) that  $\mathbf{x}$  is the set of mea-  
 2054 sured values given that the event is a signal event (signal hypothesis).
- 2055 •  $f(\mathbf{x}|b)$  is the probability density (*likelihood function*) that  $\mathbf{x}$  is the set of mea-  
 2056 sured values given that the event is a background event (background hypothe-  
 2057 sis).

2058 Figure 5.1 shows three ways to perform a classification of events for which mea-  
 2059 surements of two properties, i.e., two input variables  $x_1$  and  $x_2$ , have been performed;  
 2060 blue circles represent signal events while red triangles represent background events.  
 2061 The classification on the left is *cut-based* requiring  $x_1 < c_1$  and  $x_2 < c_2$ ; usually the  
 2062 cut values ( $c_1$  and  $c_2$ ) are chosen according to some knowledge about the event pro-  
 2063 cess. In the middle plot, the classification is performed using a linear function of  
 2064 the input variables, hence the boundary is a straight line, while in the right plot the

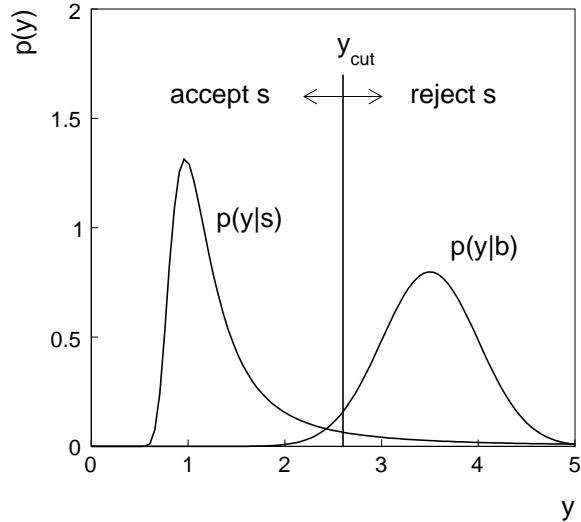
2065 the relationship between input variables is not linear thus the boundary is not linear  
 2066 either.



**Figure 5.1:** Scatter plots-MVA event classification. Distribution of two input variables  $x_1$  and  $x_2$  measured for a set of events; blue circles represent signal events and red triangles represent background events. The classification is based on cuts (left), linear boundary (center), and nonlinear boundary (right) [126]

2067 In general, the boundary can be parametrized in terms of the input variables such  
 2068 that the cut is set on the parametrization instead of on the variables, i.e.,  $y(\mathbf{x}) = y_{cut}$   
 2069 with  $y_{cut}$  being a constant; thus, the acceptance or rejection of an event is based on  
 2070 which side of the boundary the event is located. If  $y(\mathbf{x})$ , usually called *test statistic*,  
 2071 has functional form, it can be used to determine the probability distribution functions  
 2072  $p(y|s)$  and  $p(y|b)$  and then perform a test statistic with a single cut on the scalar  
 2073 variable  $y$ .

2074 Figure 5.2 shows an example of what would be the probability distribution func-  
 2075 tions under the signal and background hypotheses for a scalar test statistic with a cut  
 2076 on the classifier  $y$ . Note that the tails of the distributions indicate that some signal  
 2077 events fall in the rejection region and some background events fall on the acceptance  
 2078 region; therefore, it is convenient to define the *efficiency* with which events of a given  
 2079 type are accepted. The signal and background efficiencies are given by



**Figure 5.2:** Distributions of the scalar test statistic  $y(\mathbf{x})$  under the signal and background hypotheses. [126]

$$\varepsilon_s = P(\text{accept event}|s) = \int_A f(\mathbf{x}|s) d\mathbf{x} = \int_{-\infty}^{y_{cut}} p(y|s) dy , \quad (5.1)$$

$$\varepsilon_b = P(\text{accept event}|b) = \int_A f(\mathbf{x}|b) d\mathbf{x} = \int_{-\infty}^{y_{cut}} p(y|b) dy , \quad (5.2)$$

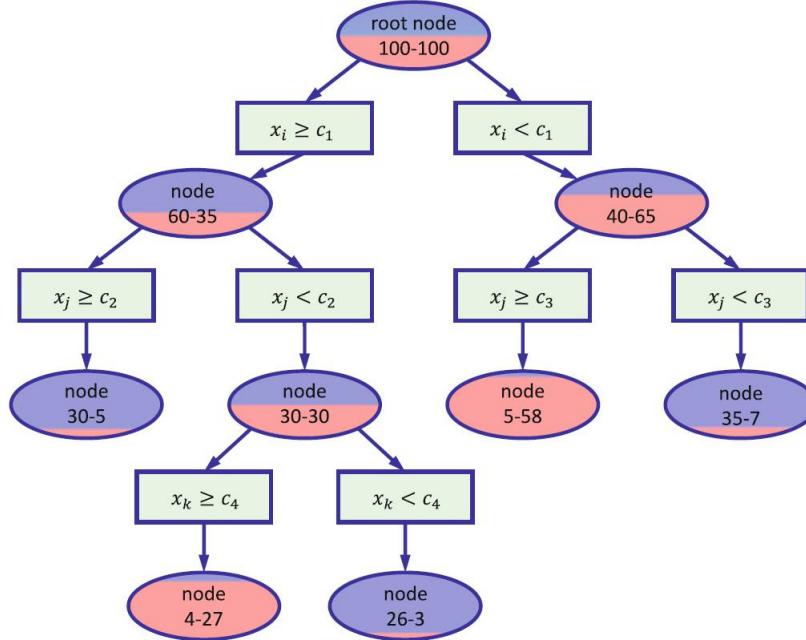
where  $A$  is the acceptance region. If the background hypothesis is the *null hypothesis* ( $H_0$ ), the signal hypothesis would be *alternative hypothesis* ( $H_1$ ); in this context, the background efficiency corresponds to the significance level of the test ( $\alpha$ ) and describes the misidentification probability, while the signal efficiency corresponds to the power of the test ( $1-\beta$ )<sup>1</sup> and describes the probability of rejecting the background hypothesis if the signal hypothesis is true. What is sought in an analysis is to maximize the power of the test relative to the significance level, i.e., set a selection with the largest possible selection efficiency and the smallest possible misidentification probability.

---

<sup>1</sup>  $\beta$  is the fraction of signal events that fall out of the acceptance region

2088 **5.1.1 Decision trees**

2089 For this thesis, the implementation of the MVA strategy, described above, is per-  
 2090 formed through decision trees by using the TMVA software package [127] included  
 2091 in the ROOT analysis framework [129]. In a simple picture, a decision tree classifies  
 2092 events according to their input variables values by setting a cut on each input variable  
 2093 and checking which events are on which side of the cut, just as proposed in the MVA  
 2094 strategy, but in addition, as a machine learning algorithm, decision trees offer the  
 2095 possibility to be trained and then perform the classification efficiently.



**Figure 5.3:** Example of a decision tree. Each node is fed with a MC sample mixing signal and background events (left-right numbers); nodes colors represent the relative number of signal/background events [128].

2096 The training or growing of a decision tree is the process where the rules for clas-  
 2097 sifying events are defined; this process is represented in Figure 5.3 and consists of  
 2098 several steps:

- 2099 • take MC samples of signal and background events and split them into two parts

2100 each; the first parts will be used in the decision tree training, while the second  
 2101 parts will be used for testing the final classifier obtained from the training.  
 2102 Each event has associated a set of input variables  $\mathbf{x} = (x_1, \dots, x_n)$  which serve  
 2103 to distinguish between signal and background events. The training sample is  
 2104 taken in at the *root node*.

- 2105     • Pick one variable, say  $x_i$ .
- 2106     • Pick one value of  $x_i$ , each event has its own value of  $x_i$ , and split the training  
     2107 sample into two subsamples  $B_1$  and  $B_2$ ;  $B_1$  contains events for which  $x_i < c_1$   
     2108 while  $B_2$  contains the rest of the training events;
- 2109     • scan all possible values of  $x_i$  and find the splitting value that provides the *best*  
     2110 classification<sup>2</sup>, i.e.,  $B_1$  is mostly made of signal events while  $B_2$  is mostly made  
     2111 of background events.
- 2112     • It is possible that variables other than the picked one produce a better classi-  
     2113 fication, hence, all the variables have to be evaluated. Pick the next variable,  
     2114 say  $x_j$ , and repeat the scan over its possible values.
- 2115     • At the end, all the variables and their values will have been scanned, the *best*  
     2116 variable and splitting value will have been identified, say  $x_1, c_1$ , and there will  
     2117 be two nodes fed with the subsamples  $B_1$  and  $B_2$ .

2118 Nodes are further split by repeating the decision process until a given number of  
 2119 final nodes is obtained, nodes are largely dominated by either signal or background  
 2120 events, or nodes have too few events to continue. Final nodes are called *leaves* and  
 2121 they are classified as signal or background leaves according to the class of the majority  
 2122 of events in them. Each *branch* in the tree corresponds to a sequence of cuts.

---

<sup>2</sup> Quality of the classification will be treated in the next paragraph.

2123        The quality of the classification at each node is evaluated through a separation  
 2124   criteria; there are several of them but the *Gini Index* ( $G$ ) is the one used in the  
 2125   decision trees trained for the analysis in this thesis.  $G$  is written in terms of the  
 2126   purity ( $P$ ), i.e., the fraction of signal events in the samples after the separation is  
 2127   made; it is given by

$$G = P(1 - P) \quad (5.3)$$

2128   note that  $P=0.5$  at the root node while  $G=0$  for pure leaves. For a node  $A$  split into  
 2129   two nodes  $B_1$  and  $B_2$  the  $G$  gain is

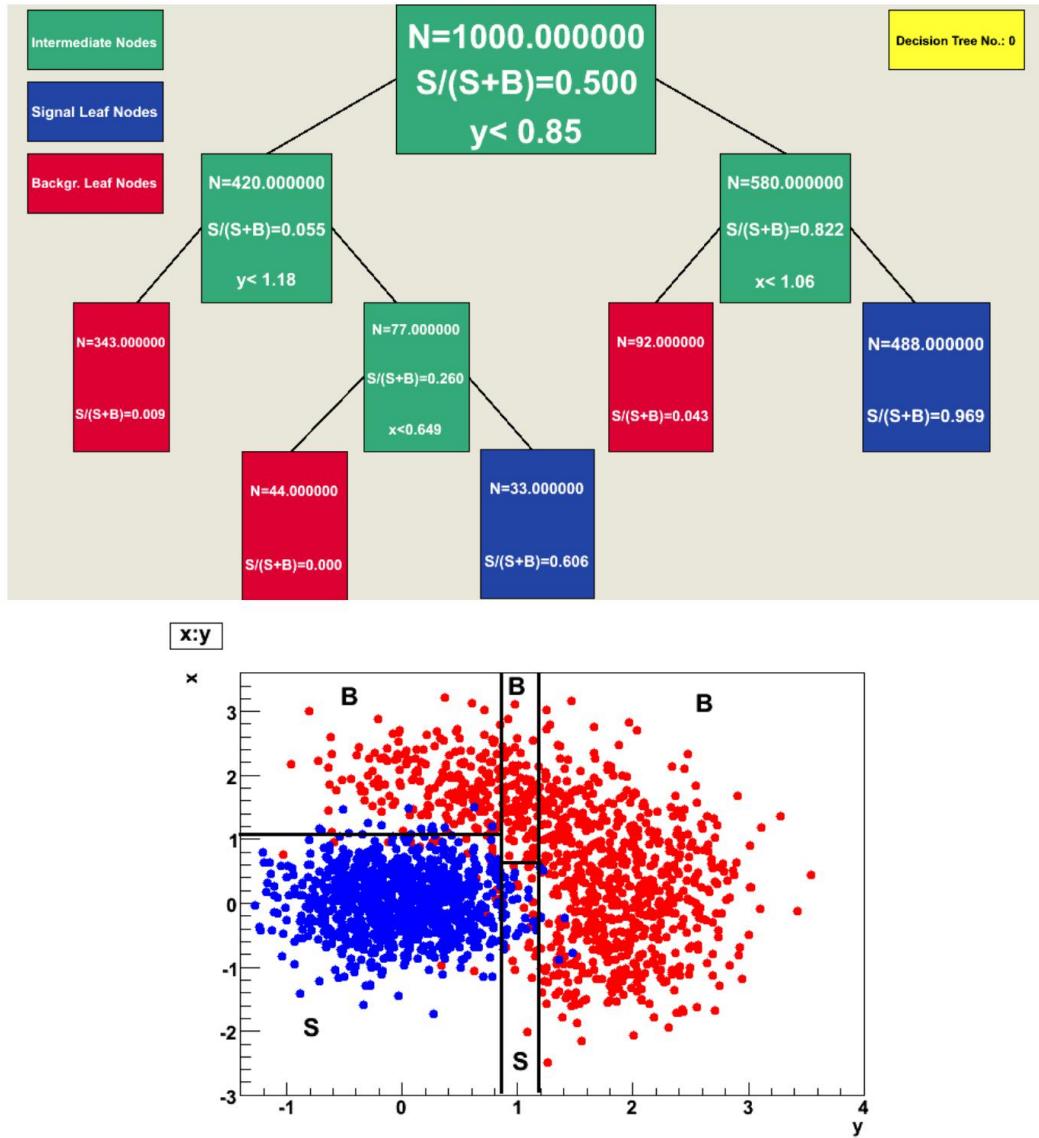
$$\Delta G = G(A) - G(B_1) - G(B_2). \quad (5.4)$$

2130        The *best* classification corresponds to that for which the gain of  $G$  is maximized;  
 2131   hence, the scanning over all the variables in an event and their values is of great  
 2132   importance.

2133        In order to provide a numerical output for the classification, events in a sig-  
 2134   nal(background) leaf are assigned an score of 1(-1) each, defining in this way the  
 2135   decision tree *classifier/weak learner* as

$$f(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \text{ in signal region,} \\ -1 & \mathbf{x} \text{ in background region.} \end{cases}$$

2136        Figure 5.4 shows an example of the classification of a sample of events, containing  
 2137   two variables, performed by a decision tree.



**Figure 5.4:** Example of a decision tree output. Each leaf, blue for signal events and red for background events, is represented by a region in the variables phase space [130].

### 2138 5.1.2 Boosted decision trees (BDT).

2139 Event misclassification occurs when a training event ends up in the wrong leaf, i.e., a  
 2140 signal event ends up in a background leaf or a background event ends up in a signal  
 2141 leaf. A way to correct it is to assign a weight to the misclassified events and train  
 2142 a second tree using the reweighted events; the event reweighting is performed by a

2143 boosting algorithm in such a way that when used in the training of a new decision  
 2144 tree the *boosted events* get correctly classified. The process is repeated iteratively  
 2145 adding a new tree to the forest and creating a set of classifiers, which are combined  
 2146 to create the next classifier; the final classifier offers more stability<sup>3</sup> and has a smaller  
 2147 misclassification rate than any individual ones. The resulting tree collection is known  
 2148 as a *boosted decision tree (BDT)*.

2149 Thus, purity of the sample is generalized to

$$P = \frac{\sum_s w_s}{\sum_s w_s + \sum_b w_b} \quad (5.5)$$

2150 where  $w_s$  and  $w_b$  are the weights of the signal and background events respectively;  
 2151 the Gini index is also generalized

$$G = \left( \sum_i^n w_i \right) P(1 - P) \quad (5.6)$$

2152 with  $n$  the number of events in the node. The final score of an event, after pass-  
 2153 ing through the forest, is calculated as the renormalized sum of all the individual  
 2154 (possibly weighted) scores; thus, high(low) score implies that the event is most likely  
 2155 signal(background).

2156 The boosting procedure, implemented in the *Gradient boosting* algorithm used in  
 2157 this thesis, produces a classifier  $F(\mathbf{x})$  which is the weighted sum of the individual  
 2158 classifiers obtained after each iteration, i.e.,

$$F(\mathbf{x}) = \sum_{m=1}^M \beta_m f(\mathbf{x}; a_m) \quad (5.7)$$

2159 where  $M$  is the number of trees in the forest. The *loss function*  $L(F, y)$  represents the

---

<sup>3</sup> Decision trees suffer from sensitivity to statistical fluctuations in the training sample which may lead to very different results with a small change in the training samples.

2160 deviation between the classifier  $F(\mathbf{x})$  response and the true value  $y$  obtained from the  
 2161 training sample (1 for signal events and -1 for background event), according to

$$L(F, y) = \ln(1 + e^{-2F(\mathbf{x})y}) \quad (5.8)$$

2162 thus, the reweighting is employed to ensure the minimization of the loss function; a  
 2163 more detailed description of the minimization procedure can be found in Reference  
 2164 [131]. The final classifier output is later used as a final discrimination variable, labeled  
 2165 as *BDT output/response*.

### 2166 5.1.3 Overtraining

2167 Decision trees offer the possibility to have as many nodes as desired in order to  
 2168 reduce the misclassification to zero (in theory); however, when a classifier is too much  
 2169 adjusted to a particular training sample, the classifier's response to a slightly different  
 2170 sample may leads to a completely different classification results; this effect is known  
 2171 as *overtraining*.

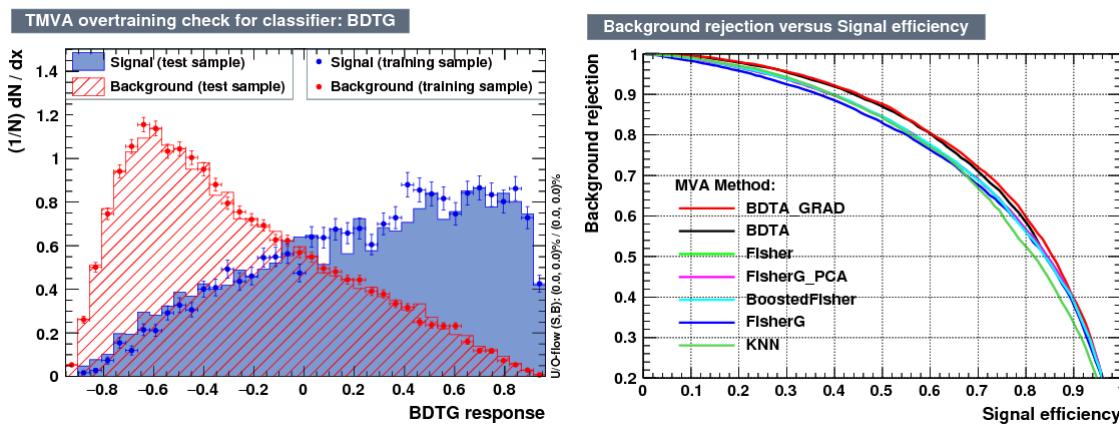
2172 An alternative to reduce the overtraining in BDTs consists in pruning the tree  
 2173 by removing statistically insignificant nodes after the tree growing is completed but  
 2174 this option is not available for BDTs with gradient boosting in the TMVA-toolkit,  
 2175 therefore, the overtraining has to be reduced by tuning the algorithm, number of  
 2176 nodes, minimum number of events in the leaves, etc. The overtraining can be evaluated  
 2177 by comparing the responses of the classifier when running over the training and  
 2178 test samples.

### 2179 5.1.4 Variable ranking

2180 BDTs have a couple of particular advantages related to the input variables; they are  
 2181 relatively insensitive to the number of input variables used in the vector  $\mathbf{x}$ . The  
 2182 ranking of the BDT input variables is determined by counting the number of times a  
 2183 variable is used to split decision tree nodes; in addition, the separation gain-squared  
 2184 achieved in the splitting and the number of events in the node are accounted by  
 2185 applying a weighting to that number. Thus, those variables with small or no power  
 2186 to separate signal and background events are rarely chosen to split the nodes, i.e., are  
 2187 effectively ignored.

2188 In addition, variables correlations play an important role for some MVA methods  
 2189 like the Fisher discriminant algorithm in which the first step consist of performing a  
 2190 linear transformation to a phase space where the correlations between variables are  
 2191 removed; in the case of BDT algorithm, correlations do not affect the performance.

### 2192 5.1.5 BDT output example



**Figure 5.5:** Left: Output distributions for the gradient boosted decision tree (BDTG) classifier using a sample of signal ( $pp \rightarrow tHq$ ) and background ( $pp \rightarrow tt$ ) events. Right: Background rejection vs signal efficiency (ROC curves) for various MVA classifiers running over the same sample used to produce the plot on the left.

2193        The left side of figure 5.5 shows the BDT output distributions for signal ( $pp \rightarrow$   
 2194       $tHq$ ) and background ( $pp \rightarrow t\bar{t}$ ) events; this plot is the equivalent to the one showed  
 2195      in Figure 5.2. A forest with 800 trees, maximum depth per tree = 3, and gradient  
 2196      boosting have been used as training parameters. The BDTG classifier offers a good  
 2197      separation power. There is a small overtraining in the signal distribution, while the  
 2198      background distribution is very well predicted which might indicate that the sample  
 2199      is composed of more background than signal events.

2200        The right side of figure 5.5 shows the background rejection vs signal efficiency  
 2201      curves for several combinations of MVA classifiers-boosting algorithms running over  
 2202      the same MC sample; these curves are known as ROC curves and give an indication  
 2203      of the performance of the classifier. In this particular example, the best performance  
 2204      is achieved with the BDTG classifier (BDTA\_GRAD), which motivate its use in this  
 2205      thesis.

## 2206      **5.2 Statistical inference**

2207      Once events are classified, the next step consists of finding the parameters that define  
 2208      the likelihood functions  $f(\mathbf{x}|s)$ ,  $f(\mathbf{x}|b)$  for signal and background events respectively.  
 2209      In general, likelihood functions depend not only on the measurements but also on  
 2210      parameters ( $\theta_m$ ) that define their shapes; the process of estimating these *unknown*  
 2211      *parameters* and their uncertainties from the experimental data is called *inference*.

2212        The statistical inference tools used in this analysis are implemented in the RooFit  
 2213      toolkit [132] and COMBINE package [133] included in the CMSSW software frame-  
 2214      work.

2215 **5.2.1 Nuisance parameters**

2216 The unknown parameter vector  $\theta$  is made of two types of parameters: those pa-  
 2217 rameters that provide information about the physical observables of interest for the  
 2218 experiment or *parameters of interest*, and the *nuisance parameters* that are not of  
 2219 a direct interest for the experiment but that need to be included in the analysis in  
 2220 order to achieve a satisfactory description of the data; they represent effects of the  
 2221 detector response like the finite resolutions of the detection systems, miscalibrations,  
 2222 and in general any source of uncertainty introduced in the analysis.

2223 Nuisance parameters can be estimated from experimental data; for instance, data  
 2224 samples from a test beam are usually employed for calibration purposes. In cases  
 2225 where experimental samples are not availables, the estimation of nuisance parameters  
 2226 makes use of dedicated simulation programs to provide the required samples.

2227 The estimation of the unknown parameters involves certain deviations from their  
 2228 true values, hence, the measurement of the nuisance parameter is written in terms  
 2229 of an estimated value, also called central value,  $\hat{\theta}$  and its uncertainty  $\delta\theta$  using the  
 2230 notation

$$\theta = \hat{\theta} \pm \delta\theta \quad (5.9)$$

2231 where the interval  $[\hat{\theta} - \delta\theta, \hat{\theta} + \delta\theta]$  is called *confidence interval*; it is usually interpreted,  
 2232 in the limit of infinite number of experiments, as the interval where the true value  
 2233 of the unknown parameter  $\theta$  is contained with a probability of 0.6827 (if no other  
 2234 convention is stated); this interval represents the area under a Gaussian distribution  
 2235 in the interval  $\pm 1\sigma$ .

2236 Conventionally, uncertainties are split into two classes: *systematic*, associated with  
 2237 the systematic effects, and *statistical*, related only to fluctuations in data and having

2238 statistical nature.

### 2239 5.2.2 Maximum likelihood estimation method

2240 The estimation of the unknown parameters that are in best agreement with the ob-  
 2241 served data is performed through a function of the data sample that returns the  
 2242 estimate of those parameters; that function is called an *estimator*. Estimators are  
 2243 usually constructed using mathematical expressions encoded in computer programs.

2244 In this thesis, the estimator used is the likelihood function  $f(\mathbf{x}|\boldsymbol{\theta})$ <sup>4</sup> which depends  
 2245 on a set of measured variables  $\mathbf{x}$  and a set of unknown parameters  $\boldsymbol{\theta}$ . The likelihood  
 2246 function for N events in a sample is the combination of all the individual likelihood  
 2247 functions, i.e.,

$$L(\boldsymbol{\theta}) = \prod_{i=1}^N f(\mathbf{x}^i|\boldsymbol{\theta}) = \prod_{i=1}^N f(x_1^i, \dots, x_n^i; \theta_1, \dots, \theta_m) \quad (5.10)$$

2248 and the estimation method used is the *Maximum Likelihood Estimation* method  
 2249 (MLE); it is based on the combined likelihood function defined by eqn. 5.10 and  
 2250 the procedure seeks for the parameter set that corresponds to the maximum value of  
 2251 the combined likelihood function, i.e., the *maximum likelihood estimator* of the un-  
 2252 known parameter vector  $\boldsymbol{\theta}$  is the function that produces the vector of *best estimators*  
 2253  $\hat{\boldsymbol{\theta}}$  for which the likelihood function  $L(\boldsymbol{\theta})$  evaluated at the measured  $\mathbf{x}$  is maximum.

2254 Usually, the logarithm of the likelihood function is used in numerical algorithm  
 2255 implementations in order to avoid underflow the numerical precision of the computers  
 2256 due to the product of small likelihoods. In addition, it is common to minimize the  
 2257 negative logarithm of the likelihood function, therefore, the negative log-likelihood

---

<sup>4</sup> analogue to the likelihood functions described in previous sections

2258 function is

$$F(\boldsymbol{\theta}) = -\ln L(\boldsymbol{\theta}) = -\sum_{i=1}^N f(\mathbf{x}^i | \boldsymbol{\theta}). \quad (5.11)$$

2259 The minimization process is performed by the software MINUIT [134] imple-  
 2260 mented in the ROOT analysis framework. In case of data samples with large number  
 2261 of measurements, the computational resources necessary to calculate the likelihood  
 2262 function are too big; therefore, the parameter estimation is performed using binned  
 2263 distributions of the variables of interest for which the *binned likelihood function* is  
 2264 given by

$$L(\mathbf{x}|r, \boldsymbol{\theta}) = \prod_{i=1} \frac{(r \cdot s_i(\boldsymbol{\theta}) + b_i(\boldsymbol{\theta}))^{n_i}}{n_i!} e^{-r \cdot s_i(\boldsymbol{\theta}) - b_i(\boldsymbol{\theta})} \prod_{j=1} \frac{1}{\sqrt{2\pi}\sigma_{\theta_j}^2} e^{-(\theta_j - \theta_{0,j})^2/2\sigma_{\theta_j}^2}, \quad (5.12)$$

2265 with  $s_i$  and  $b_i$  the expected number of signal and background yields for the bin  $i$ ,  $n_i$  is  
 2266 the observed number of events in the bin  $i$  and  $r = \sigma/\sigma_{SM}$  is the signal strength. Note  
 2267 that the number of entries per bin follows a Poisson distribution. The effect of the  
 2268 nuisance parameters have been included in the likelihood function through Gaussian  
 2269 distributions that models the nuisance. The three parameters,  $r$ ,  $s_i$  and  $b_i$  are jointly  
 2270 fitted to estimate the value of  $r$ .

## 2271 5.3 Upper limits

2272 In this analysis, two hypotheses are considered; the background only hypothesis  
 2273 ( $H_0(b)$ ) and the signal plus background hypothesis ( $H_1(s+b)$ ), i.e., the sample of  
 2274 events is composed of background only events ( $r=0$ ) or it is a mixture of signal plus  
 2275 background events ( $r=1$ ). The exclusion of one hypothesis against the other means  
 2276 that the observed data sample better agrees with  $H_0$  or rather with  $H_1$ . In order  
 2277 to discriminate these hypotheses, a test statistic is constructed on the basis of the

2278 likelihood function evaluated for each of the hypothesis.

2279 The *Neyman-Pearson* lemma [135] states that the test statistic that provides the  
 2280 maximum power for  $H_1$  for a given significance level (background misidentification  
 2281 probability  $\alpha$ ), is given by the ratio of the likelihood functions  $L(\mathbf{x}|H_1)$  and  $L(\mathbf{x}|H_0)$ ;  
 2282 however, in order to use that definition it is necessary to know the true likelihood  
 2283 functions, which in practice is not always possible. Approximate functions obtained  
 2284 by numerical methods, like the BDT method described above, have to be used, so  
 2285 that the *profile likelihood* test statistic is defined by

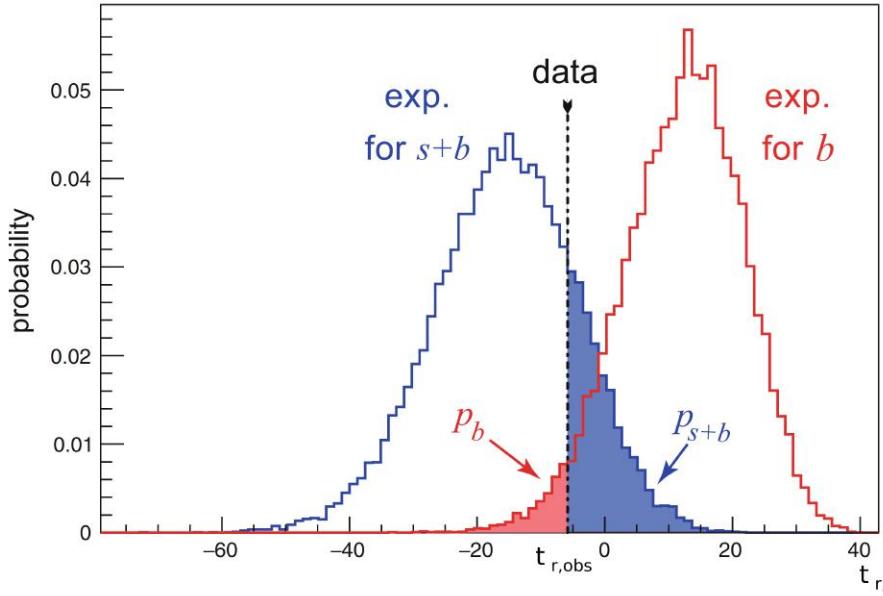
$$\lambda(\mathbf{r}) = \frac{L(\mathbf{x}|r, \hat{\boldsymbol{\theta}}(r))}{L(\mathbf{x}|\hat{r}, \hat{\boldsymbol{\theta}})}, \quad (5.13)$$

2286 where,  $\hat{r}$  and  $\hat{\boldsymbol{\theta}}$  maximize the likelihood function, and  $\hat{\boldsymbol{\theta}}$  maximizes the likelihood  
 2287 function for a given value of the signal strength modifier  $r$ . In practice, the test  
 2288 statistic  $t_r$

$$t_r = -2\ln\lambda(r) \quad (5.14)$$

2289 is used to evaluate the presence of signal in the sample, since the minimum of  $t_r$  at  
 2290  $r = \hat{r}$  suggests the presence of signal with signal strength  $\hat{r}$ . The uncertainty interval  
 2291 for  $r$  is determined by the values of  $r$  for which  $t_r = +1$ .

2292 The expected probability density function (p.d.f)  $f(t_r|r, \boldsymbol{\theta})$  of the test statistic  $t_r$   
 2293 can be obtained numerically by generating MC samples where one hypothesis,  $H_0(b)$   
 2294 or  $H_1(s+b)$ , is assumed; thus, MC samples contain the possible values of  $t_r$  obtained  
 2295 from *pseudo-experiments* as shown in Figure 5.6. The probability that  $t_r$  takes a value  
 2296 equal or greater than the observed value ( $t_{r,obs}$ ) when a signal with a signal modifier  
 2297  $r$  is present in the data sample, is called the *p-value* of the observation; it can be  
 2298 calculated using



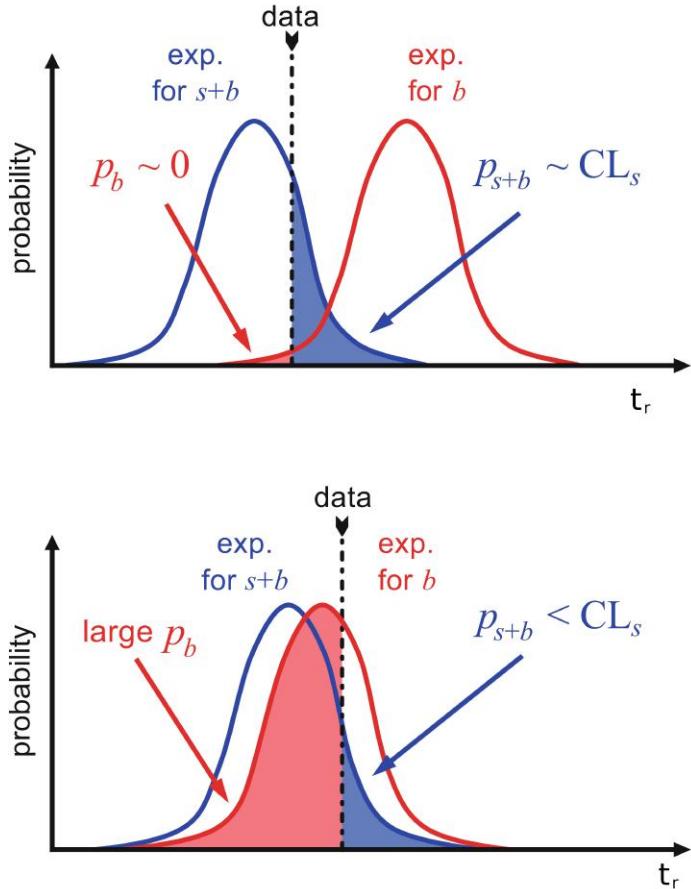
**Figure 5.6:**  $t_r$  p.d.f. from MC pseudo experiments assuming  $H_0$  (red) and  $H_1$  (blue). The black dashed line shows the value of the test statistic as measured from data. Adapted from Reference [128].

$$p_r = \int_{t_{r,obs}}^{\infty} f(t'_r | r, \boldsymbol{\theta}) dt'_r, \quad (5.15)$$

thus,  $p_r < 0.05$  means that, for that particular value of  $r$ ,  $H_1$  could be excluded at 95% Confidence Level (CL). The corresponding background-only p-value is given by

$$1 - p_b = \int_{t_{r,obs}}^{\infty} f(t'_r | 0, \boldsymbol{\theta}) dt'_r, \quad (5.16)$$

If the  $t_r$  p.d.f.s for both hypotheses are well separated, as shown in the top side of Figure 5.7, the experiment is sensitive to the presence of signal in the sample. If the signal presence is small, both p.d.f.s will be largely overlapped (bottom of Figure ??) and either the signal hypothesis could be rejected with not enough justification because the experiment is not sensitive to the signal or a fluctuation of the background could be misinterpreted as presence of signal with the corresponding rejection of the



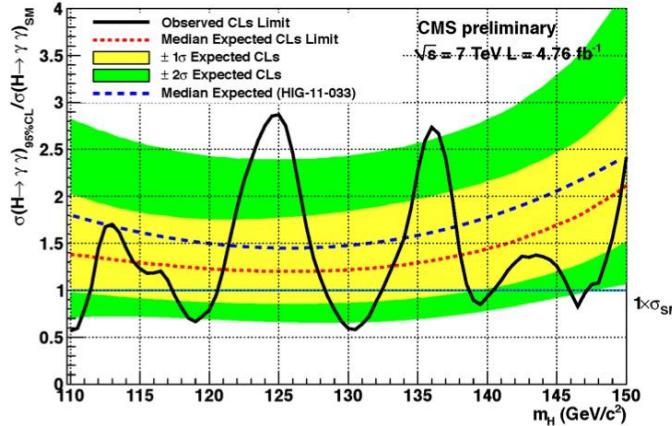
**Figure 5.7:**  $CL_s$  limit illustration. When the test statistic p.d.f. for the two hypotheses  $H_0$  and  $H_1$  are well separated (top) and when they are largely overlapped (bottom). Adapted from Reference [128].

2307 background-only hypothesis. These issues are corrected by using the modified p-  
2308 value [136]

$$p'_r = \frac{p_r}{1 - p_b} \equiv CL_s. \quad (5.17)$$

2309 If  $H_1$  is true, then  $p_b$  is small,  $CL_s \simeq p_r$  and  $H_0$  is rejected; if there is large  
2310 overlap and a statistical fluctuation causes that  $p_b$  is large, then both numerator and  
2311 denominator in Eqn. 5.17 become small but  $CL_s$  would allow the rejection of  $H_1$   
2312 even if there is poor sensitivity to signal.

2313        The upper limit of the parameter of interest  $r^{up}$  is determined by excluding the  
 2314   range of values of  $r$  for which  $CL_s(r, \theta)$  is lower than the confidence level desired,  
 2315   normally 90% or 95%, e.g, scanning over  $r$  and finding the value for which  $p_r'^{up} =$   
 2316   0.05. The expected upper limit can be calculated using pseudo-experiments based on  
 2317   the background-only hypothesis and obtaining a distribution for  $r_{ps}^{up}$ ; the median of  
 2318   that distribution corresponds to the expected upper limit, while the  $\pm 1\sigma$  and  $\pm 2\sigma$   
 2319   deviations correspond to the values of the distribution that defines the 68% and 95%  
 2320   of the area under the distribution centered in the median. It is usual to present all  
 2321   the information about the expected and observed limits in the so-called *Brazilian-flag*  
 2322   *plot* as the one showed in Figure 5.8. The solid line represent the observed  $CL_s$



**Figure 5.8:** Brazilian flag plot of CMS experiment limits for Higgs boson decaying to photons [137].

## 2323        5.4 Asymptotic limits

2324   As said before, the complexity of the likelihood functions, the construction of test  
 2325   statistics, and the calculation of the limits and their uncertainties is not always man-  
 2326   ageable and requires extensive computational resources; in order to overcome those  
 2327   issues, asymptotic approximations for likelihood-based test statistics, like the ones

described in previous sections, have been developed [138, 139] using Wilks' theorem.  
Asymptotic approximations replace the construction of the test statistics p.d.f.s using  
MC pseudo-experiments, with the approximate calculation of the test statistics p.d.f.s  
by employing the so-called *Asimov dataset*.

The Asimov dataset is defined as the dataset that produce the true values of the  
nuisance parameters when it is used to evaluate the estimators for all the parameters;  
it is obtained by setting the values of the variables in the dataset to their expected  
values [139].

Limits calculated by using the asymptotic approximation and the Asimov dataset  
are know as *asymptotic limits*.

2338 **Chapter 6**

2339 **Search for production of a Higgs**

2340 **boson and a single top quark in**

2341 **multilepton final states in pp**

2342 **collisions at  $\sqrt{s} = 13$  TeV**

2343 **6.1 Introduction**

2344 The Higgs boson discovery, supported on experimental observations and theoretical  
2345 predictions made about the SM, gives the clue of the way in that elementary parti-  
2346 cles acquire mass through the Higgs mechanism; therefore, knowing the Higgs mass,  
2347 the Higgs-vector boson and Higgs-fermion couplings can be tested. In order to test  
2348 the Higgs-top coupling, several measurements have been performed, as stated in the  
2349 chapter 1, but they are limited in sensitivity to measure the square of the coupling.

2350 The production of a Higgs boson in association with a single top quark ( $tH$ ) not  
2351 only offers access to the sign of the coupling, but also, to the CP phase of the Higgs

2352    couplings.

2353    This chapter presents the search for the associated production of a Higgs boson  
 2354    and a single top quark ( $tHq$ ) events, focusing on leptonic signatures provided by the  
 2355    Higgs decay modes to  $WW$ ,  $ZZ$ , and  $\tau\tau$ ; the 13 TeV dataset produced in 2016, with  
 2356    an integrated luminosity of  $35.9\text{fb}^{-1}$ , is used.

2357    As shown in Section 1.5, the SM cross section of  $tHq$  process is affected by a  
 2358    destructive interference between two contributions (see Figure 1.15), where the Higgs  
 2359    couples to either the W boson or the top quark; however, if the sign of the Higgs-  
 2360    top coupling is flipped with respect to the SM prediction, a large enhancement of  
 2361    the cross section occurs, making this analysis sensitive to such deviation. A second  
 2362    process, where the Higgs boson and top quark are accompanied by a W boson ( $tHW$ )  
 2363    has similar behavior, albeit with a weaker interference pattern and lower contribution  
 2364    to the cross section, therefore, a combination of both processes would increase the  
 2365    sensitivity to the sign of the coupling; in this analysis both contributions are combined  
 2366    and referred to as  $tH$  channel. A third contribution comes from  $t\bar{t}H$  process. The  
 2367    purpose of this analysis is to investigate the exclusion of the presence of the  $tH +$   
 2368     $t\bar{t}H$  processes in the SM under the assumption of the anomalous Higgs-top coupling  
 2369    modifier ( $\kappa_t = -1$ ). The analysis exploits signatures with two leptons of the same sign  
 2370    ( $2lss$ ) channel and three leptons ( $3l$ ) channel in the final state.

2371    Constraints on the sign of the Higgs-top coupling ( $y_t$ ) have been derived from the  
 2372    decay rate of Higgs boson to photon pairs [50] and from the cross section for associated  
 2373    production of Higgs and Z bosons via gluon fusion [141], with recent results disfavoring  
 2374    negative signs of the coupling [44, 59, 142], although the negative sign coupling have  
 2375    not been completely excluded.

2376    The analysis presented here, expands previous analyses performed at 8 TeV [143,  
 2377    144] and searches for associated production of  $t\bar{t}$  pair and a Higgs boson in the mul-

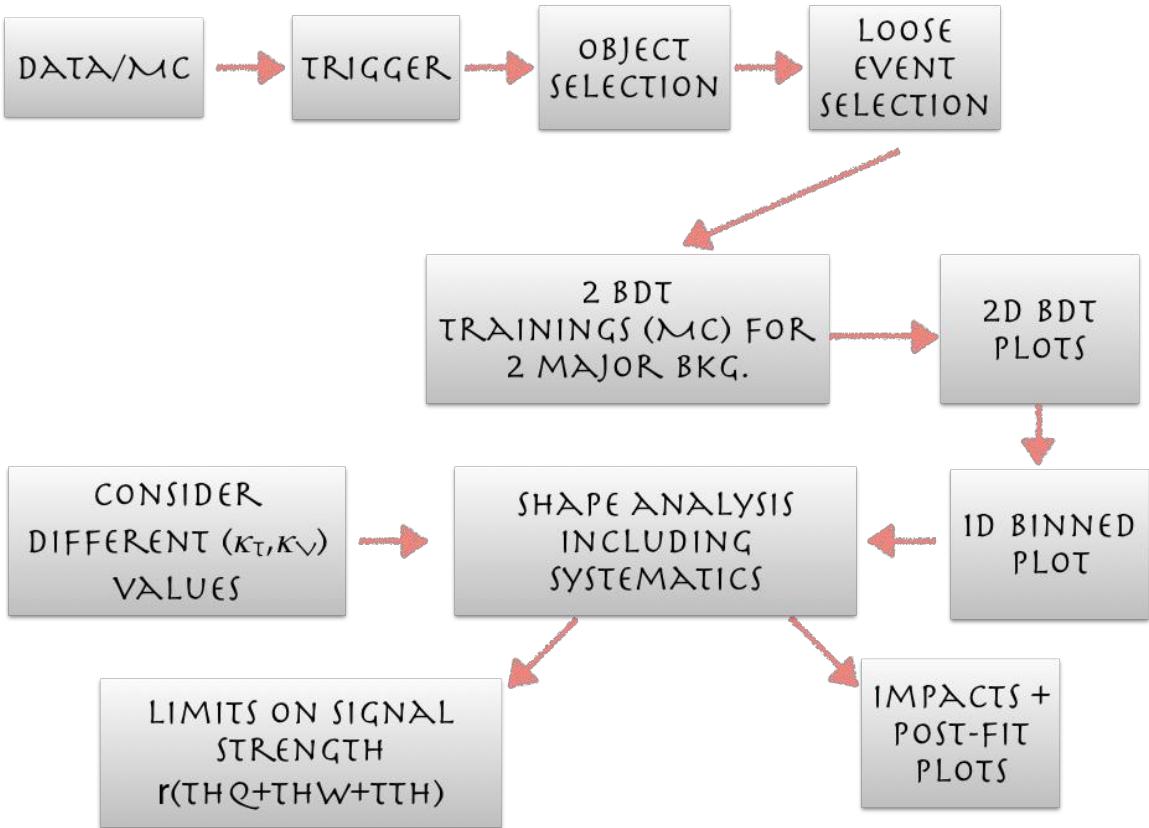
2378 tilepton final state channel [145]; it also complements searches in  $H \rightarrow b\bar{b}$  [146].

2379 The first sections present the characteristic  $tHq$  signature as well as the expected  
 2380 backgrounds. The MC samples, data sets, and the physics object definitions are then  
 2381 described; after, the background predictions, the signal extraction, the statistical  
 2382 treatment of the selected events and the discussion of the systematic uncertainties  
 2383 are described. The final section presents the results for the exclusion limits as a  
 2384 function of the ratio of  $\kappa_t$  and the dimensionless modifier of the Higgs-vector boson  
 2385 coupling  $\kappa_V$ .

2386 The analysis is designed to efficiently identify and select prompt leptons from on-  
 2387 shell W and Z boson decays and to reject non-prompt leptons from  $b$  quark decays  
 2388 and spurious lepton signatures from hadronic jets. Events are then selected in the  
 2389  $2lss$  and  $3l$  channels, and are required to contain hadronic jets, some of which must  
 2390 be consistent with  $b$  quark hadronization. Finally, the signal yield is extracted by  
 2391 simultaneously fitting the output of two dedicated multivariate discriminants, trained  
 2392 to separate the  $tHq$  signal from the two dominant backgrounds, in all categories. The  
 2393 fit result is then used to set an upper limit on the combined  $t\bar{t}H + tH$  production  
 2394 cross section, as a function of the relative coupling strengths of Higgs-top quark and  
 2395 Higgs-Vector boson. Figure 6.1 shows an schematic overview of the analysis strategy  
 2396 workflow.

2397 With respect to the 8 TeV analysis, the object selections have been adjusted for  
 2398 the updated LHC running conditions at 13 TeV, the lepton identification has been  
 2399 improved, and more powerful multivariate analysis techniques are used for the signal  
 2400 extraction.

2401 The analysis has been made public by CMS as a Physics Analysis Summary [147]  
 2402 combining the result for the three lepton and two lepton same-sign channels; the  
 2403 content present in this chapter is based on that document and on References [145,149]

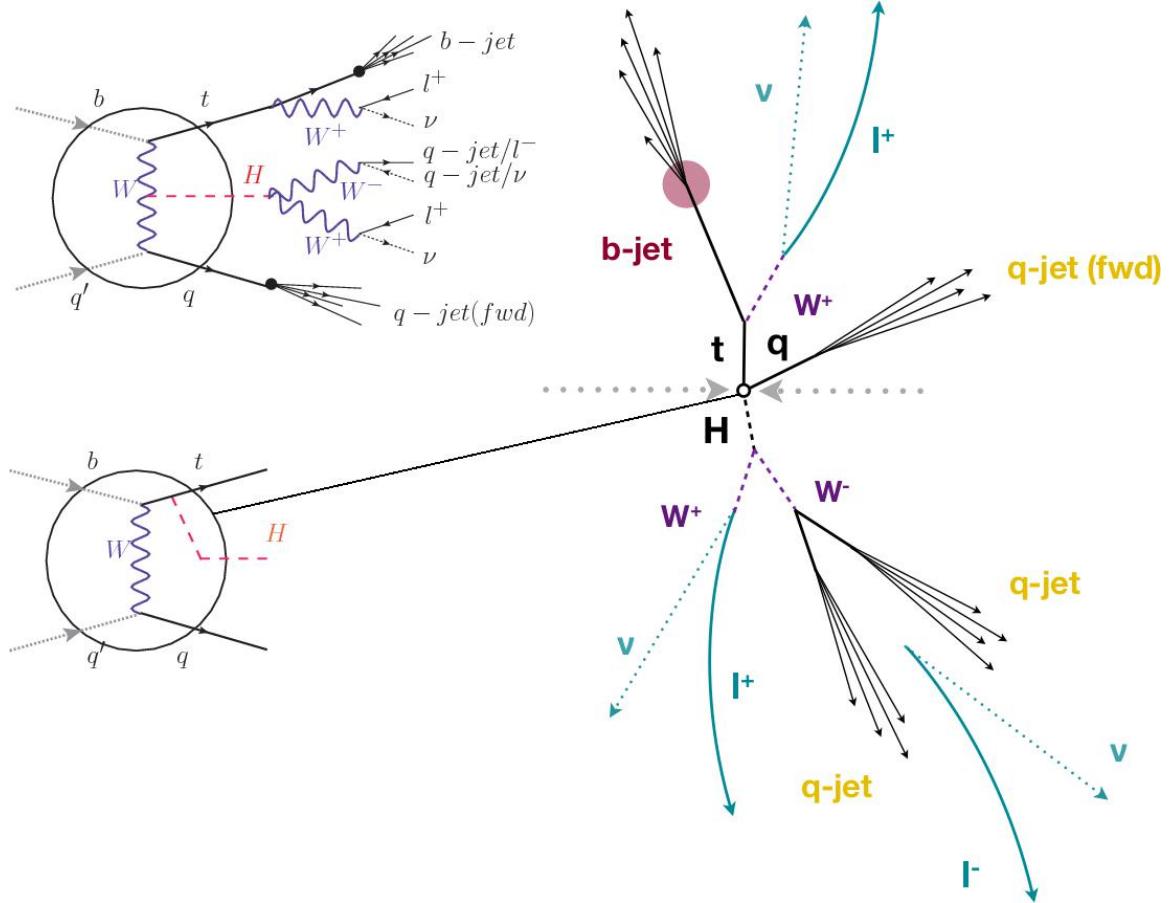


**Figure 6.1:** A schematic overview of the analysis workflow. Based on sets of optimized physics object definitions and selection criteria, signal and background events in a data sample are discriminated. The discrimination is performed by a BDT, previously trained using MC samples of the dominant backgrounds, using discriminant variables based on the  $b$ -jet multiplicity, the activity in the forward region of the detector, and the kinematic properties of leptons. The  $CL_s$  limits on the combined  $t\bar{t}H + tH$  production cross section, as a function of the relative coupling strengths are calculated.

unless other Reference is stated. Currently, an effort to turn the analysis into a paper combining the multilepton and  $H \rightarrow b\bar{b}$  is ongoing.

## 6.2 $tHq$ signature

In order to select events of  $tHq$  process, its features are translated into a set of selection rules; Figure 6.2 shows the Feynman diagram and a schematic view of the



**Figure 6.2:**  $tHq$  event signature. Left: Feynman diagram including the whole evolution up to the final state for the case of the Higgs boson emitted by the  $W$  boson (top); Feynman diagram for the case where the Higgs boson is emitted by the top quark. Right: Schematic view as it would be seen in the detector; the circle in the Feynman diagrams on the left corresponds to the circle in the center of the schematic view as indicated by the line connecting them. In the  $2lss$  channel, one of the  $W$  bosons from the Higgs boson decays to two light-quark jets while in the  $3l$  channel both  $W$  bosons decay to leptons.

2409  $tHq$  process from the  $pp$  collision to the final state configuration. A single top quark  
 2410 is produced accompanied by a light quark, denoted as  $q$ ; this light quark is produced  
 2411 predominantly in the forward region of the detector. The Higgs boson can be either  
 2412 emitted by the exchanged  $W$  boson or directly by the singly produced top quark.

2413 Due to their high masses/short lifetimes, top quark and Higgs boson decay after  
 2414 their production within the detector. The Higgs boson is required to decay into a  $W$

2415 boson pair<sup>1</sup>. The top quark almost always decays into a bottom quark and a W boson,  
 2416 as encoded in the CMK matrix. The W bosons are required to decay leptonically  
 2417 either all the three in the  $3l$  channel or the pair with equal electrical charge in the  
 2418  $2lss$  channel case;  $\tau$  leptons are not reconstructed separately and only their leptonic  
 2419 decays into either electrons or muons are considered in this analysis.

2420 In summary, the signal process is characterized by a the final state with

- 2421 • one light-flavored forward jet,
  - 2422 • one central b-jet,
  - 2423 •  $2lss$  channel → two leptons of the same sign, two neutrinos and two light (often  
 2424 soft) jets,
  - 2425 •  $3l$  channel → three leptons, three neutrinos and no central light-flavored jets,
- 2426 The presence of neutrinos is inferred from the presence of MET.

## 2427 6.3 Background processes

2428 The background processes are those that can mimic the signal signature or at least  
 2429 can be reconstructed as signal as a result of certain circumstances. The backgrounds  
 2430 can be classified as

- 2431 • irreducible backgrounds: where genuine prompt leptons are produced in on-  
 2432 shell W and Z boson decays; they can be reliably estimated directly from MC  
 2433 simulated events, using higher-order cross sections or data control regions for  
 2434 the overall normalization.

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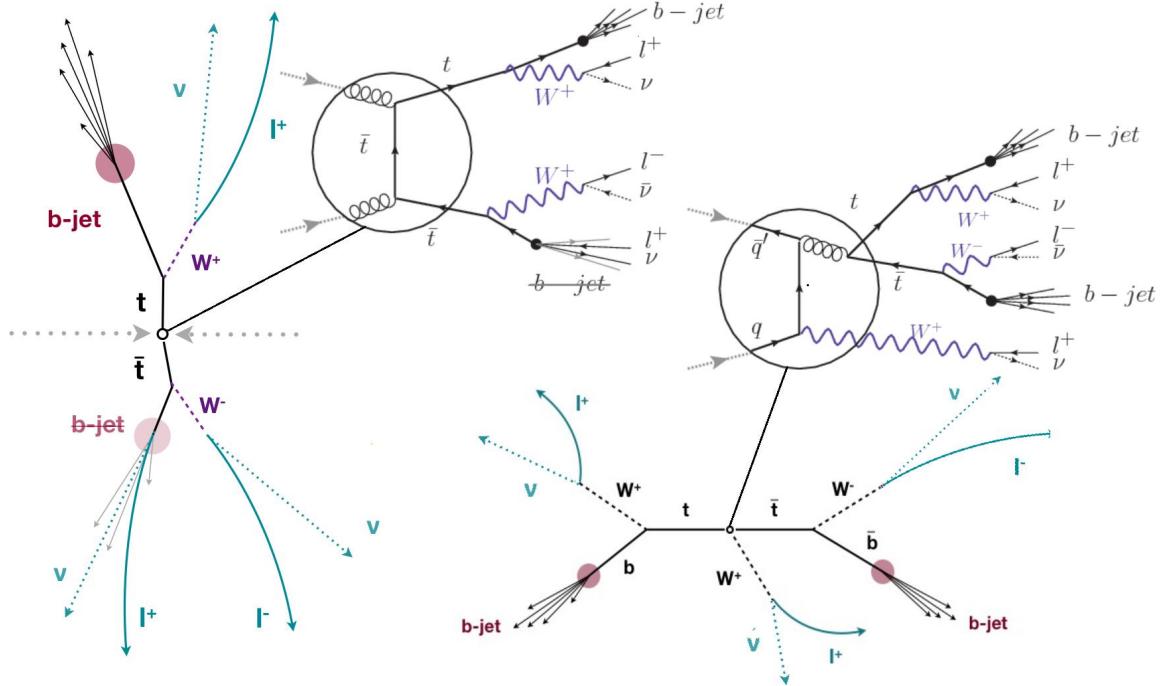
<sup>1</sup> ZZ and  $\tau\tau$  decays are also include in the analysis but they are not separately reconstructed

2435     • reducible backgrounds: where at least one of the leptons is *non-prompt*, i.e.,  
 2436       produced within a hadronic jet; genuine leptons from heavy flavor decays and  
 2437       misreconstructed jets, also known as *mis-ID leptons* are considered non-prompt  
 2438       leptons or or *fake leptons* as well as electrons from photon conversions. These  
 2439       non-prompt leptons leave tracks and hits in the detection systems as would a  
 2440       prompt lepton, but evaluation the correlation of those hits with nearby jets  
 2441       could be a way of removing them. The misassignment of electron charge in  
 2442       processes like  $t\bar{t}$  or Drell-Yan, represents an additional source of background,  
 2443       but it is relevant only for the  $2lss$  channel. Reducible backgrounds are not well  
 2444       predicted by simulation, hence, they are estimated using data-driven methods.

2445       The main sources of background events for  $tHq$  process are  $t\bar{t}$  process and  $t\bar{t}V(V =$   
 2446        $W, Z, \gamma$ ) processes. Figure 6.3 shows the signature for  $t\bar{t}$  and  $t\bar{t}W$  processes.

2447       The largest contribution to irreducible backgrounds comes from  $t\bar{t}W$  and  $t\bar{t}Z$   
 2448       processes for which the number of ( $b-$ )jets (( $b-$ )jet multiplicity) is higher than that  
 2449       of the signal events, while for other contributing background events,  $WZ$ ,  $ZZ$ , and  
 2450       rare SM processes like  $W^\pm W^\pm qq$ ,  $t\bar{t}t\bar{t}$ ,  $tZq$ ,  $tZW$ ,  $WWW$ ,  $WWZ$ ,  $WZZ$ ,  $ZZZ$ ,  
 2451       the ( $b-$ )jet multiplicity is lower compared to that of the signal events. None of the  
 2452       irreducible backgrounds present activity in the forward region of the detector.

2453       On the side of the reducible backgrounds, the largest contribution comes from the  
 2454        $t\bar{t}$  events which have a very similar signature to the signal events but does no present  
 2455       activity in the forward region of the detector either; A particular feature of the  $t\bar{t}$   
 2456       events is their charge-symmetry, which is different from the characteristics of signal  
 2457       events.



**Figure 6.3:**  $t\bar{t}$  (left) and  $t\bar{t}W$  (right) events signature as they would be seen in the detector; the Feynman diagrams including the whole evolution up to the final state are also showed. The  $t\bar{t}$  process signature is very similar to that of the signal process with one fake lepton and no forward activity. The  $t\bar{t}W$  process presents a higher b-jet multiplicity compared to the signal process, a prompt lepton and no forward activity.

## 2458 6.4 Data and MC Samples

### 2459 6.4.1 Full 2016 data set

2460 The data set used in this analysis was collected by the CMS experiment during 2016,  
 2461 while running at  $\sqrt{s} = 13$  TeV, and corresponds to a total integrated luminosity  
 2462 of  $35.9 \text{ fb}^{-1}$ . Only periods when the CMS magnet was on were considered when  
 2463 selecting the data samples; that corresponds to the 23Sep2016 (Run B to G) and  
 2464 PromptReco (Run H) versions of the datasets.

2465 Multilepton final states with either two same-sign leptons or three leptons tar-  
 2466 get the case where the Higgs boson decays to a pair of W bosons,  $\tau$  leptons, or Z  
 2467 bosons, and where the top quark decays leptonically, hence, the SingleElectron,

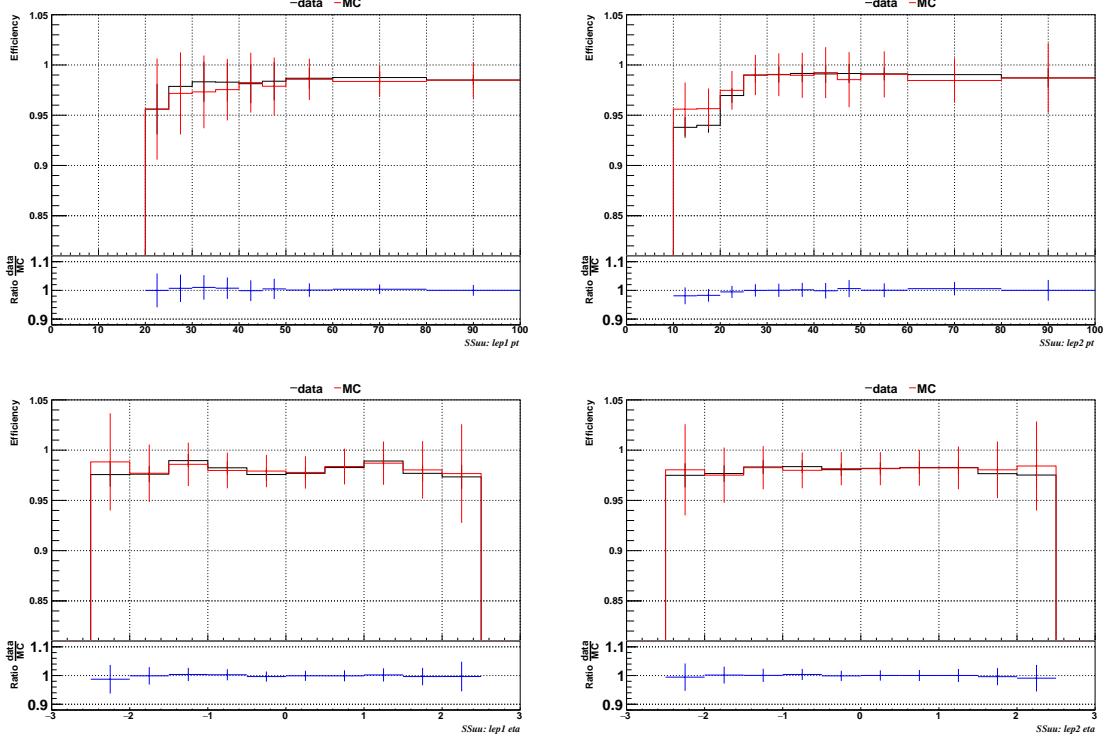
2468 SingleMuon, DoubleEG, MuonEG, DoubleMuon dataset (see Table A.1) compose the  
 2469 full dataset. The certified luminosity sections are selected using the golden JSON file  
 2470 defined by the CMS experiment [148].

## 2471 6.4.2 Triggers

2472 The events considered are those online-reconstructed events triggered by one, two, or  
 2473 three leptons. Single-lepton triggers are included in order to boost the acceptance  
 2474 of events where the  $p_T$  of the sub-leading lepton falls below the threshold of the  
 2475 double-lepton triggers. The trigger efficiency is increased by including double-lepton  
 2476 triggers in the  $3l$  category, and single-lepton triggers in all categories; it is possible  
 2477 given the logical “or” of the trigger decisions of all the individual triggers in a given  
 2478 category. Table A.2 shows the lowest-threshold non-prescaled triggers present in the  
 2479 High-Level Trigger (HLT) menus for both Monte-Carlo and data in 2016.

## 2480 Trigger efficiency scale factors

2481 Trigger efficiency describes the ability of events to pass the trigger requirements. It  
 2482 is measured in simulated events using generator information given that there is no  
 2483 trigger bias with the MC sample. Measuring the trigger efficiency in data requires a  
 2484 more elaborated procedure; first, select a set of events collected by a trigger that is  
 2485 uncorrelated with the lepton triggers such that the selected events form an unbiased  
 2486 sample. In this analysis, that uncorrelated trigger is a MET trigger. Second step  
 2487 is looking for candidate events with exactly two good leptons (exactly three good  
 2488 leptons for the  $3l$  channel). Finally, measure the efficiency for the candidate events to  
 2489 pass the logical “or” of triggers being considered in a given event category as defined  
 2490 in Table A.2.

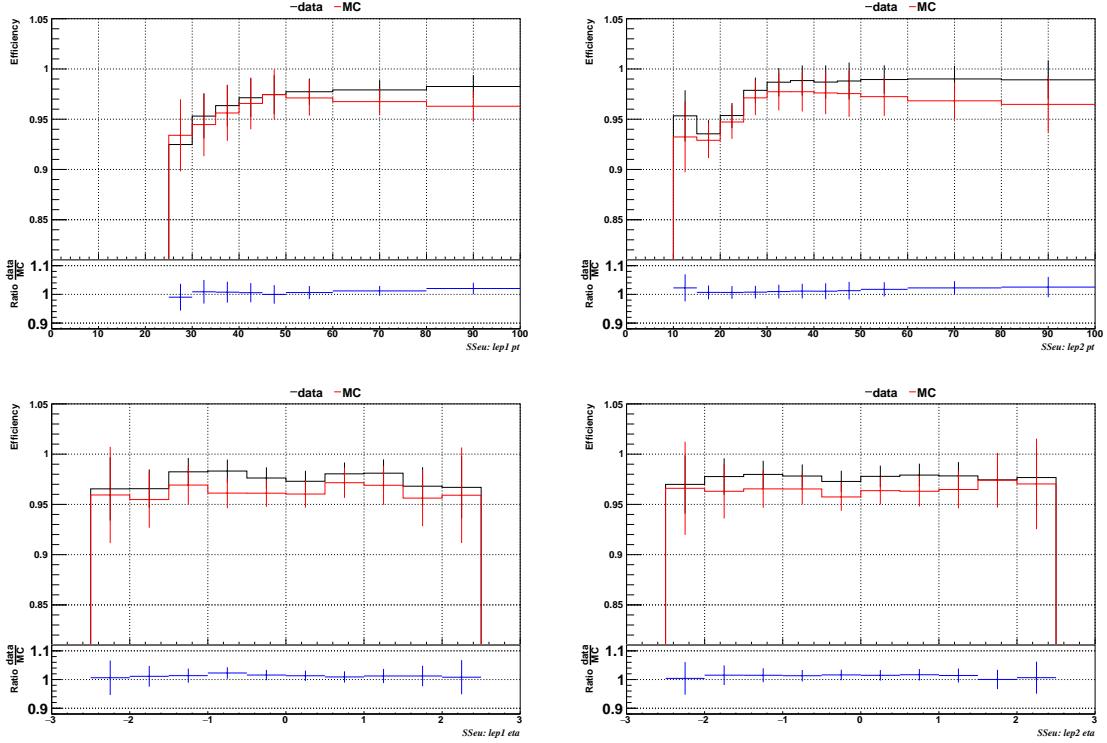


**Figure 6.4:** Comparison between data and MC trigger efficiencies in the same-sign  $\mu\mu$  category, as a function of the  $p_T$  (top) and  $\eta$  (bottom) of the leading lepton (left) and the sub-leading lepton (right) [149].

Category	Scale Factor
ee	$1.01 \pm 0.02$
e $\mu$	$1.01 \pm 0.01$
$\mu\mu$	$1.00 \pm 0.01$
3l	$1.00 \pm 0.03$

**Table 6.1:** Trigger efficiency scale factors and associated uncertainties, shown here rounded to the nearest percent.

2491 Comparisons between the data and MC efficiencies for each category, showed in  
 2492 Figures 6.4, 6.5, and 6.6, reveal that they are in good agreement; the difference is  
 2493 corrected by applying scale factors derived from the ratio between both efficiencies.  
 2494 Applied flat scale factors in each category are shown in Table 6.1; they have been  
 2495 inherited from Reference [149].

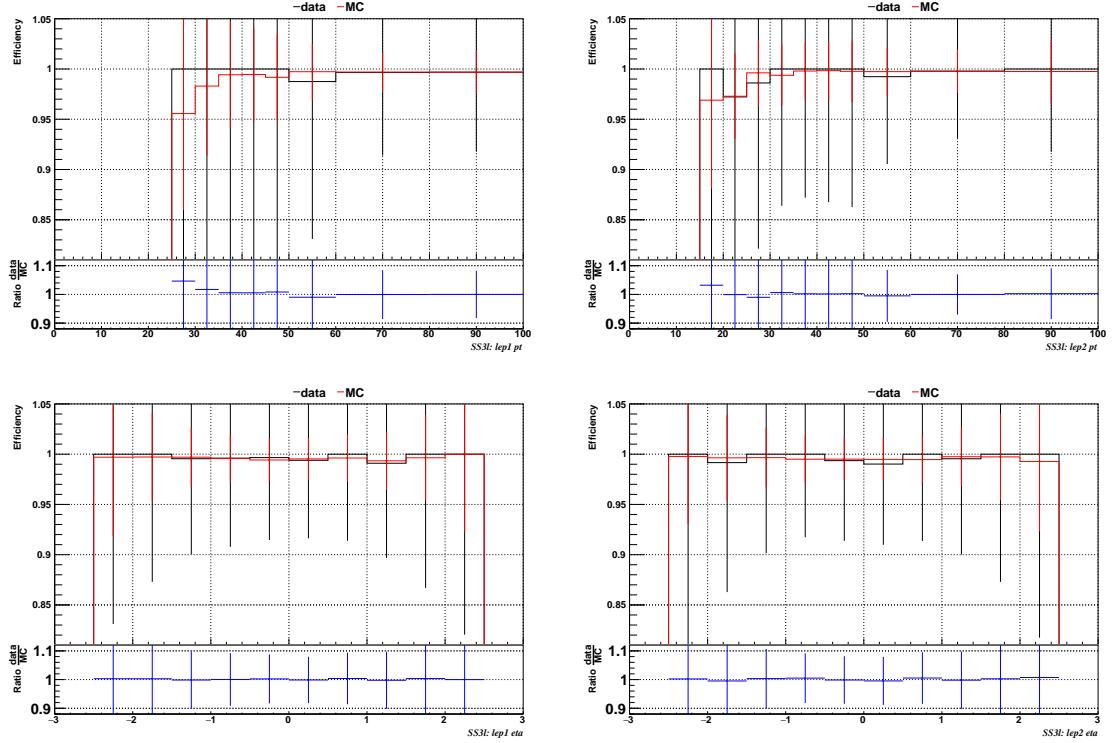


**Figure 6.5:** Comparison between data and MC trigger efficiencies in the same-sign  $e\mu$  category as a function of the  $p_T$  (top) and  $\eta$  (bottom) of the leading lepton (left) and the sub-leading lepton (right) [149].

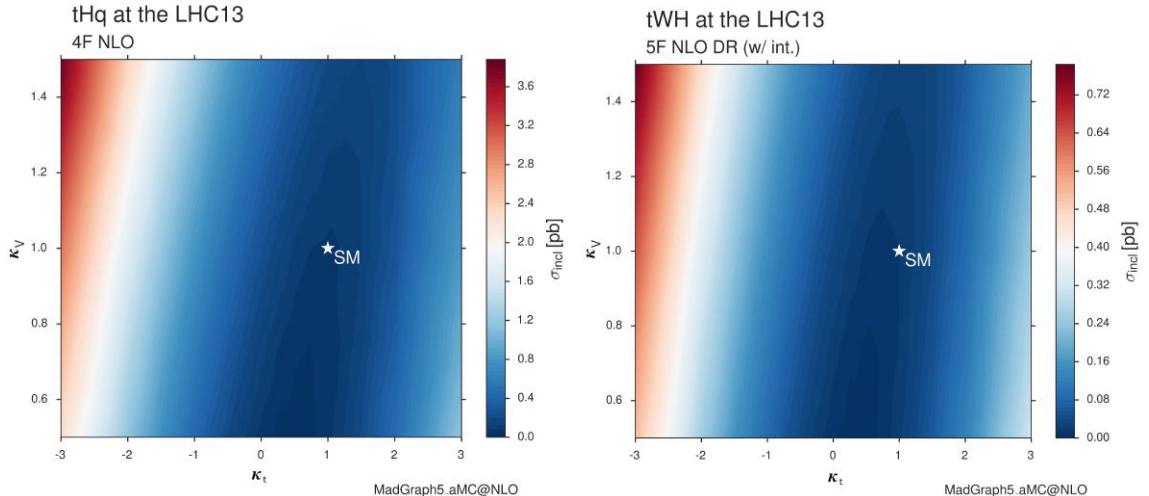
### 2496 6.4.3 MC samples

2497 Current event generators allow the adjustment of the kinematics of the generated  
 2498 events, based on an event-wise reweighting; in this way, several generation parameters  
 2499 phase spaces can be explored according to the experimental interests. The signal  
 2500 samples used in this analysis were generated in such a way that not only the case  $\kappa_t$   
 2501  $= -1$ , but an extended range of  $\kappa_t$  and  $\kappa_V$  values may be investigated.

2502  $tHq$  and  $tHW$  cross section in the  $\kappa_t$ - $\kappa_V$  phase space are shown in Figure 6.7. As  
 2503 said in section 3.1, the  $tHq$  sample was generated using the 4F scheme which provides  
 2504 a better description of the additional  $b$  quark from the initial gluon splitting, while the  
 2505  $tHW$  sample was generated using the 5F scheme in order to remove its interference



**Figure 6.6:** Comparison between data and MC trigger efficiencies in the  $3l$  category, as a function of the  $p_T$  (top) and  $\eta$  (bottom) of the leading lepton (left) and the sub-leading lepton (right) [149].



**Figure 6.7:**  $tHq$  and  $tHW$  cross section in the  $\kappa_t$ - $\kappa_V$  phase space [150].

2506 with  $t\bar{t}H$  at LO.

2507 **MC signal samples**

2508 The two signal samples,  $tHq$  and  $tHW$ , correspond to the `RunIISummer16MiniAODv2`  
 2509 campaign produced with `CMSW_80X`; they were produced with `MG5_aMC@NLO`  
 2510 (version 5.2.2.3), in LO mode at  $\sqrt{s} = 13$  TeV, and are normalized to NLO cross sec-  
 2511 tions (see Table 6.2). The Higgs boson is assumed to be SM-like except for the values  
 2512 of its couplings to the top quark and W boson. Each sample was generated with a set  
 2513 of event weights corresponding to 51 different values of  $(\kappa_t, \kappa_V)$  couplings, accessible  
 2514 in terms of LHE event weights as shown in Table A.3; however, the main interest is  
 2515 the  $(\kappa_t = -1, \kappa_V = 1)$  case.

Sample	$\sigma$ [pb]	BF
<code>/THQ_Hincl_13TeV-madgraph-pythia8_TuneCUETP8M1/</code>	0.7927	0.324
<code>/THW_Hincl_13TeV-madgraph-pythia8_TuneCUETP8M1/</code>	0.1472	1.0
<code>/tTHJetToNonbb_M125_13TeV_amcatnloFXFX_madspin_pythia8_mWCutfix/</code>	0.2151	1.0

2516 **Table 6.2:** MC signal samples used in this analysis; cross section and branching fraction  
 2517 are also listed [150].

2516 The  $t\bar{t}H$  sample was produced using `AMC@NLO` interfaced to `PYTHIA 8` for  
 2517 the parton shower, and is scaled to NLO cross sections. The  $t\bar{t}H$  cross section depends  
 2518 quadratically on  $\kappa_t$ ; however, in contrast to the  $tHq$  and  $tHW$  samples, the scaling  
 2519 is not performed during the sample generation process but in the analysis code since  
 2520 it was decided to include the  $t\bar{t}H$  process as a part of the signal in the course of the  
 2521 analysis.

2522 **MC background samples**

2523 Several MC generators were used to generate the samples of the background processes.  
 2524 The dominant background sources ( $t\bar{t}$ ,  $t\bar{t}W$ ,  $t\bar{t}Z$ ) were produced using `AMC@NLO`

2525 interfaced to PYTHIA8, and are scaled to NLO cross sections. Other minor back-  
 2526 ground processes are simulated using POWHEG interfaced to PYTHIA, or bare  
 2527 PYTHIA as stated in the sample names in Table A.4. Pileup interactions are in-  
 2528 cluded in the simulation in order to reflect the observed multiplicity in data; the  
 2529 simulated events are weighted according to the actual pileup in data, estimated from  
 2530 the measured bunch-to-bunch instantaneous luminosity and the total inelastic cross  
 2531 section, 69.2 mb. All events are finally passed through a full simulation of the CMS  
 2532 detector using GEANT4, and reconstructed using the same algorithms as used for  
 2533 the data.

## 2534 **6.5 Object Identification**

2535 In this section, the specific definitions of the physical objects in terms of the recon-  
 2536 struction parameters are presented; thus, the provided details summarize and com-  
 2537 plement the descriptions presented in previous chapters. The object reconstruction  
 2538 and selection strategy used in this thesis are inherited from the analyses in Refer-  
 2539 ences [145, 149].

### 2540 **6.5.1 Lepton reconstruction and identification**

2541 Two types of leptons are defined in this analysis: *signal leptons* are those coming from  
 2542  $W, Z$  and  $\tau$  decays which usually are isolated from other particles; *background leptons*  
 2543 are defined as leptons produced in  $b$ -jet hadron decays, light-jets misidentification,  
 2544 and photon conversions.

2545 The process of reconstruction and identification of electron and muon candidates  
 2546 was described in chapter3, hence, the identification variables used in order to retain

2547 the highest possible efficiency for signal leptons while maximizing the rejection of  
 2548 background leptons are listed and described in the following sections <sup>2</sup>.

2549 The identification variables include not only observables related directly to the re-  
 2550 constructed leptons themselves, but also to the clustered energy deposits and charged  
 2551 particles in a cone around the lepton direction (jet-related variables); an initial loose  
 2552 preselection of leptons candidates is performed and then an MVA discriminator, re-  
 2553 ferred to as *lepton MVA* discriminator, is used to distinguish signal leptons from  
 2554 background leptons.

## 2555 Muons

2556 The Physics Objects Groups (POG) at CMS, are in charge of studying and defining  
 2557 the set of selection criteria applied on the course of reconstruction and identification  
 2558 of particles. These selection criteria are implemented in the CMS framework in the  
 2559 form of several object identification working points according to the strength of the  
 2560 requirements.

2561 The muon candidates are reconstructed by combining information from the tracker  
 2562 system and the muon detection system of CMS detector and the POG defined three  
 2563 working points for muon identification *MuonID* [153];

- 2564     • *POG Loose Muon ID* is a particle identified as a muon by the PF event re-  
     2565 construction and also reconstructed either as a global-muon or as an arbitrated  
     2566 tracker-muon. This identification criteria is designed to be highly efficient for  
     2567 prompt muons and for muons from heavy and light quark decays; it can be com-  
     2568 plemented by applying impact parameter cuts in analyses with prompt muon  
     2569 signals.

---

<sup>2</sup> The studies performed to optimize the identification are far from the scope of this thesis,  
 therefore, only general descriptions are provided

- 2570     • *POG Medium Muon ID* is a Loose muon with additional track-quality and  
 2571       muon-quality (spatial matching between the individual measurements in the  
 2572       tracker and the muon system) requirements. This identification criteria is de-  
 2573       signed to be highly efficient in the separation of the muons coming from decay  
 2574       in flight of heavy quarks and muons coming from B meson decays as well as  
 2575       prompt muons. An additional category *MVA Prompt ID* is defined in this iden-  
 2576       tification criteria directed to discriminated muons from B mesons and prompt  
 2577       muons (from W,Z and  $\tau$  decays). The Medium ID provides the same fake rate as  
 2578       the Tight Muon ID but a higher efficiency on prompt and B-decays muons. [154]
- 2579     • *POG Tight Muon ID* is a global muon with additional muon-quality require-  
 2580       ments Tight Muon ID selects a subset of the PF muons.

2581       Only muons within the muon system acceptance  $|\eta| < 2.4$  and minimum  $p_T$  of 5  
 2582       GeV are considered.

## 2583     **Electrons**

2584       Electrons are reconstructed using information from the tracker and from the electro-  
 2585       magnetic calorimeter and identified by an MVA algorithm (*MVA eID* discriminant)  
 2586       using the shape of the calorimetric shower variables like the shape in  $\eta$  and  $\phi$ , the clus-  
 2587       ter circularity, widths along  $\eta$  and  $\phi$ ; track-cluster matching variables like  $E_{tot}/p_{in}$ ,  
 2588        $E_{Ele}/p_{out}$ ,  $\Delta\eta_{in}$ ,  $\Delta\eta_{out}$ ,  $\Delta\phi_{in}$ ,  $1/E - 1/p$ ; and track quality variables like  $\chi^2$  of the  
 2589       GSF tracks, the number of hits used by the GSF filter [155].

2590       A loose selection based on  $\eta$ -dependent cuts on this discriminant is used to prese-  
 2591       lect electron candidates, the full shape of the discriminant is used in the lepton MVA  
 2592       selection to separate signal leptons from background leptons (described in Section  
 2593       6.5.1).

2594 In order to reject electrons from photon conversions, electron candidates with  
 2595 missing hits in the pixel tracker layers or matched to a conversion secondary vertex  
 2596 are discarded. Electrons are selected for the analysis if they have  $p_T > 7$  GeV and  
 2597 are located within the tracker system acceptance region ( $|\eta| < 2.5$ ).

2598 **Lepton vertexing and pile-up rejection**

2599 The impact parameter in the transverse plane  $d_0$ , impact parameter along the  $z$ -  
 2600 axis  $d_z$ , and the impact parameter significance in the detector space  $SIP_{3D}$ , are  
 2601 considered to perform the identification and rejection of pile-up, misreconstructed  
 2602 tracks, and background leptons from b-hadron decays; pile-up and misreconstructed  
 2603 track mitigation is achieved by imposing loose cuts on the impact parameter variables.  
 2604 The full shape of those variables is used in a lepton MVA classifier to achieve the best  
 2605 separation between the signal and the background leptons.

2606 **Lepton isolation**

2607 PF is able to recognize leptons from two different sources: on one side, leptons from  
 2608 the decays of heavy particles, such as W and Z bosons, which are normally isolated in  
 2609 space from the hadronic activity in the event; on the other side, leptons from decays  
 2610 of hadrons and jets misidentified as leptons, which are not isolated as the former. For  
 2611 highly boosted systems, like the lepton and the  $b$ -jet generated in the semileptonic  
 2612 decay of a boosted top, the decay products tend to be more closer and sometimes they  
 2613 even overlap; thus, the PF standard definition of isolation in terms of the separation  
 2614  $\Delta R$  between lepton candidates ( $l$ ) and other PF objects ( $i$ ) in the  $\eta$ - $\phi$  plane,

$$\Delta R = \sqrt{(\eta^l - \eta^i)^2 + (\phi^l - \phi^i)^2} < 0.3 \quad (6.1)$$

which considers all the neutral, charged hadrons and photons in a cone around the leptons, is refocused to the local isolation of the leptons through the mini-isolation  $I_{mini}$  [156] defined as the sum of particle flow candidates  $p_T$  within a cone around the lepton, corrected for the effects of pileup and divided by the lepton  $p_T$

$$I_{mini} = \frac{\sum_R p_T(h^\pm) - \max\left(0, \sum_R p_T(h^0) + p_T(\gamma) - \rho \mathcal{A}\left(\frac{R}{0.3}\right)^2\right)}{p_T(l)} \quad (6.2)$$

where  $\rho$  is the pileup energy density,  $h^\pm, h^0, \gamma, l$ , represent the charged hadron, neutral hadrons, photons, and the lepton, respectively. The radius  $R$  of the cone depends on the  $p_T$  of the lepton according to

$$R = \frac{10\text{GeV}}{\min(\max(p_T(l), 50\text{GeV}), 200\text{GeV})}, \quad (6.3)$$

The  $p_T$  dependence of the cone size allows for greater signal efficiency. Setting a cut on  $I_{mini}$  below a given threshold ensures that the lepton is locally isolated, even in boosted systems. The effect of pileup is mitigated using the so-called effective area correction  $\mathcal{A}$  listed in Table 6.3.

$ \eta $ range	$\mathcal{A}(e)$ neutral/charged	$\mathcal{A}(\mu)$ neutral/charged
0.0 - 0.8	0.1607 / 0.0188	0.1322 / 0.0191
0.8 - 1.3	0.1579 / 0.0188	0.1137 / 0.0170
1.3 - 2.0	0.1120 / 0.0135	0.0883 / 0.0146
2.0 - 2.2	0.1228 / 0.0135	0.0865 / 0.0111
2.2 - 2.5	0.2156 / 0.0105	0.1214 / 0.0091

**Table 6.3:** Effective areas, for electrons and muons used to mitigate the effect of pileup by using the so-called effective area correction.

A loose cut on  $I_{mini}$  is applied to pre-select the muon and electron candidates; however, the full shape is used in the lepton MVA discriminator when performing the signal lepton selection.

2629 **Jet-related variables**

2630 In order to reject misidentified leptons from  $b$ -jets, mostly coming from  $t\bar{t}$ +jets,  
 2631 Drell-Yan+jets, and W+jets events, the vertexing and isolation described in previous  
 2632 sections are complemented with additional variables related to the closest recon-  
 2633 structed jet to the lepton, i.e., the PF jets reconstructed<sup>3</sup> around the leptons with  
 2634  $\Delta R = \sqrt{(\eta^l - \eta^{jet})^2 + (\phi^l - \phi^{jet})^2} < 0.5$ . The identification variables used in the lep-  
 2635 ton MVA discriminator are the ratio  $p_T^l/p_T^{jet}$ , the CSV b-tagging discriminator value  
 2636 of the jet, the number of charged tracks of the jet, and the relative  $p_T$  given by

$$p_T^{rel} = \frac{(\vec{p}_{jet} - \vec{p}_l) \cdot \vec{p}_l}{\|\vec{p}_{jet} - \vec{p}_l\|}. \quad (6.4)$$

2637 **LeptonMVA discriminator**

2638 Electrons and muons passing the basic selection process described above are referred  
 2639 to as *loose leptons*. Additional discrimination between signal leptons and background  
 2640 leptons is crucial considering that the rate of  $t\bar{t}$  production is much larger than the  
 2641 signal, hence, an overwhelming background from  $t\bar{t}$  production is present. To maxi-  
 2642 mally exploit the available information in each event to that end, the dedicated lepton  
 2643 MVA discriminator, based on a boosted decision tree (BDT) algorithm, has been built  
 2644 so that all the identification variables can be used together.

2645 The lepton MVA discriminator training is performed using simulated signal Loose  
 2646 leptons from the  $t\bar{t}H$  MC sample and fake leptons from the  $t\bar{t}$  +jets MC sample,  
 2647 separately for muons and electrons. The input variables used include vertexing, iso-  
 2648 lation and jet-related variables, the  $p_T$  and  $\eta$  of the lepton, the electron MVA eID  
 2649 discriminator and the muon segment-compatibility variables. An additional require-  
 2650 ment known as *tight-charge* requirement, is imposed by comparing two independent

---

<sup>3</sup> Charged hadrons from PU vertices are not removed prior to the jet clustering.

measurement of the charge, one from the ECAL supercluster and the other from the tracker; thus, the consistency in the measurements of the electron charge is ensured so that events with a wrong electron charge assignment are rejected; this variable is particularly used in the  $2lss$  channel to suppress opposite-sign events for which the charge of one of the leptons has been mismeasured. The tight-charge requirement for muons is represented by the requirement of a consistently well measured track transverse momentum given by  $\Delta p_T/p_T < 0.2$ . Leptons are selected for the final analysis if they pass a given threshold of the BDT output, and are referred to as *tight leptons* in the following.

The validation of the lepton MVA algorithm and the lepton identification variables is performed using data in various control regions; the details about that validation are not discussed here but can be found in Reference [149].

### Selection definitions

Electron and muon object identification is defined in three different sets of selections criteria; the *Loose*, *Fakeable Object*, and *Tight* selection. These three levels of selection are designed to serve for event level vetoes, the fake rate estimation application region (see Section 6.7.2), and the final signal selection, respectively. The  $p_T$  of fakeable objects is defined as  $0.85 \times p_T(\text{jet})$ , where the jet is the one associated to the lepton object. This mitigates the dependence of the fake rate on the momentum of the fakeable object and thereby improves the precision of the method.

Tables 6.4 and 6.5 list the full criteria for the different selections of muons and electrons.

In addition to the previously defined requirements for jets, they are required to be separated from any lepton candidates passing the fakeable object selections by  $\Delta R > 0.4$ .

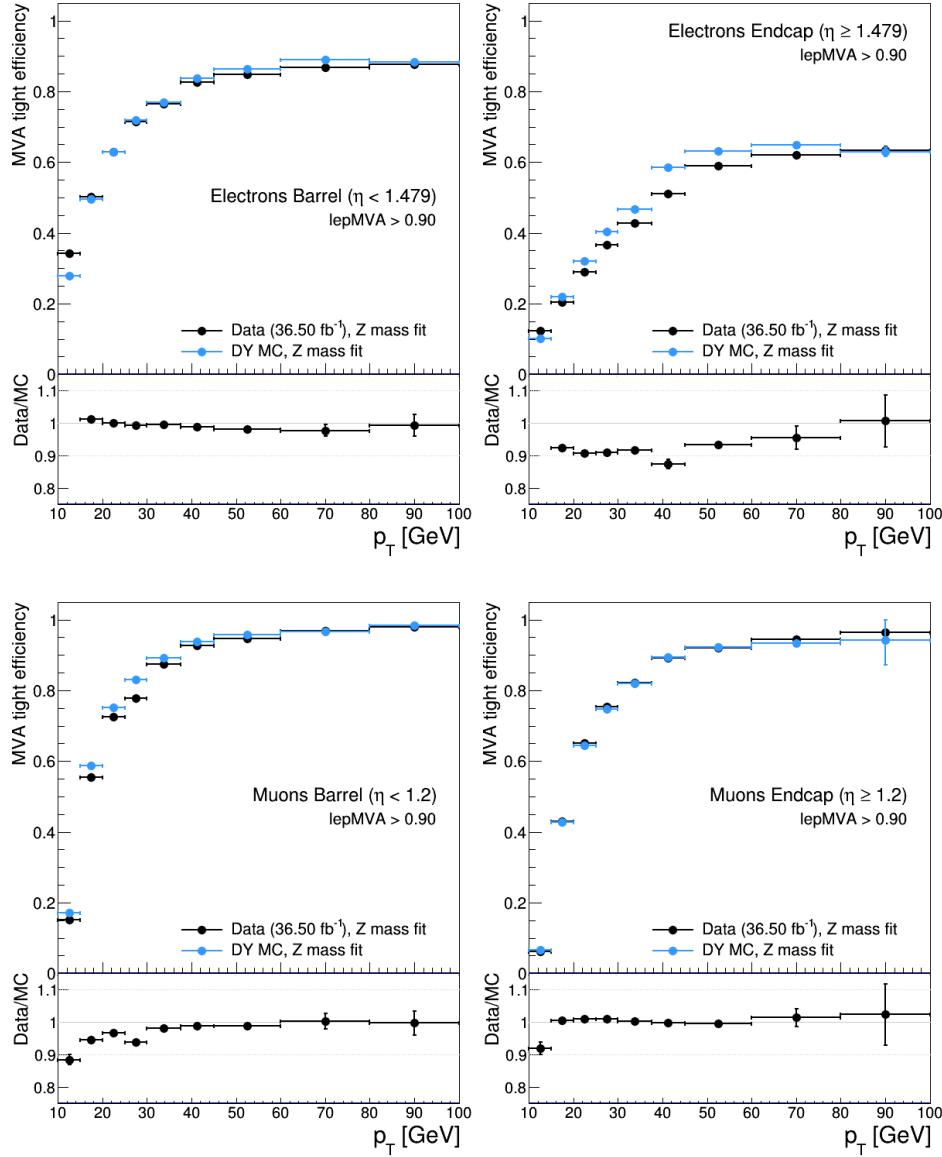
Cut	Loose	Fakeable object	Tight
$ \eta  < 2.4$	✓	✓	✓
$p_T$	$> 5\text{GeV}$	$> 15\text{GeV}$	$> 15\text{GeV}$
$ d_{xy}  < 0.05$ (cm)	✓	✓	✓
$ d_z  < 0.1$ (cm)	✓	✓	✓
$\text{SIP}_{3D} < 8$	✓	✓	✓
$I_{\text{mini}} < 0.4$	✓	✓	✓
is Loose Muon	✓	✓	✓
jet CSV	—	$< 0.8484$	$< 0.8484$
is Medium Muon	—	—	✓
tight-charge	—	—	✓
lepMVA $> 0.90$	—	—	✓

**Table 6.4:** Requirements on each of the three muon selections. In the cases where the cut values change between the selections, those values are listed in the table. Otherwise, whether the cut is applied is indicated.

Cut	Loose	Fakeable Object	Tight
$ \eta  < 2.5$	✓	✓	✓
$p_T$	$> 7\text{GeV}$	$> 15\text{GeV}$	$> 15\text{GeV}$
$ d_{xy}  < 0.05$ (cm)	✓	✓	✓
$ d_z  < 0.1$ (cm)	✓	✓	✓
$\text{SIP}_{3D} < 8$	✓	✓	✓
$I_{\text{mini}} < 0.4$	✓	✓	✓
MVA eID $> (0.0, 0.0, 0.7)$	✓	✓	✓
$\sigma_{in\eta} < (0.011, 0.011, 0.030)$	—	✓	✓
H/E $< (0.10, 0.10, 0.07)$	—	✓	✓
$\Delta\eta_{in} < (0.01, 0.01, 0.008)$	—	✓	✓
$\Delta\phi_{in} < (0.04, 0.04, 0.07)$	—	✓	✓
$-0.05 < 1/E - 1/p < (0.010, 0.010, 0.005)$	—	✓	✓
$p_T^{\text{ratio}}$	—	$> 0.5^\dagger / -$	—
jet CSV	—	$< 0.3^\dagger / < 0.8484$	$< 0.8484$
tight-charge	—	—	✓
conversion rejection	—	—	✓
Number of missing hits	$< 2$	$= 0$	$= 0$
lepton MVA $> 0.90$	—	—	✓

**Table 6.5:** Criteria for each of the three electron selections. In cases where the cut values change between selections, those values are listed in the table. Otherwise, whether the cut is applied is indicated. In some cases, the cut values change for different  $\eta$  ranges. These ranges are  $0 < |\eta| < 0.8$ ,  $0.8 < |\eta| < 1.479$ , and  $1.479 < |\eta| < 2.5$  and the respective cut values are given in the form (value<sub>1</sub>, value<sub>2</sub>, value<sub>3</sub>). For the two  $p_T^{\text{ratio}}$  and CSV rows, the cuts marked with a  $\dagger$  are applied to leptons that fail the lepton MVA cut, while the loose cut value is applied to those that pass the lepton MVA cut.

2676 **6.5.2 Lepton selection efficiency**



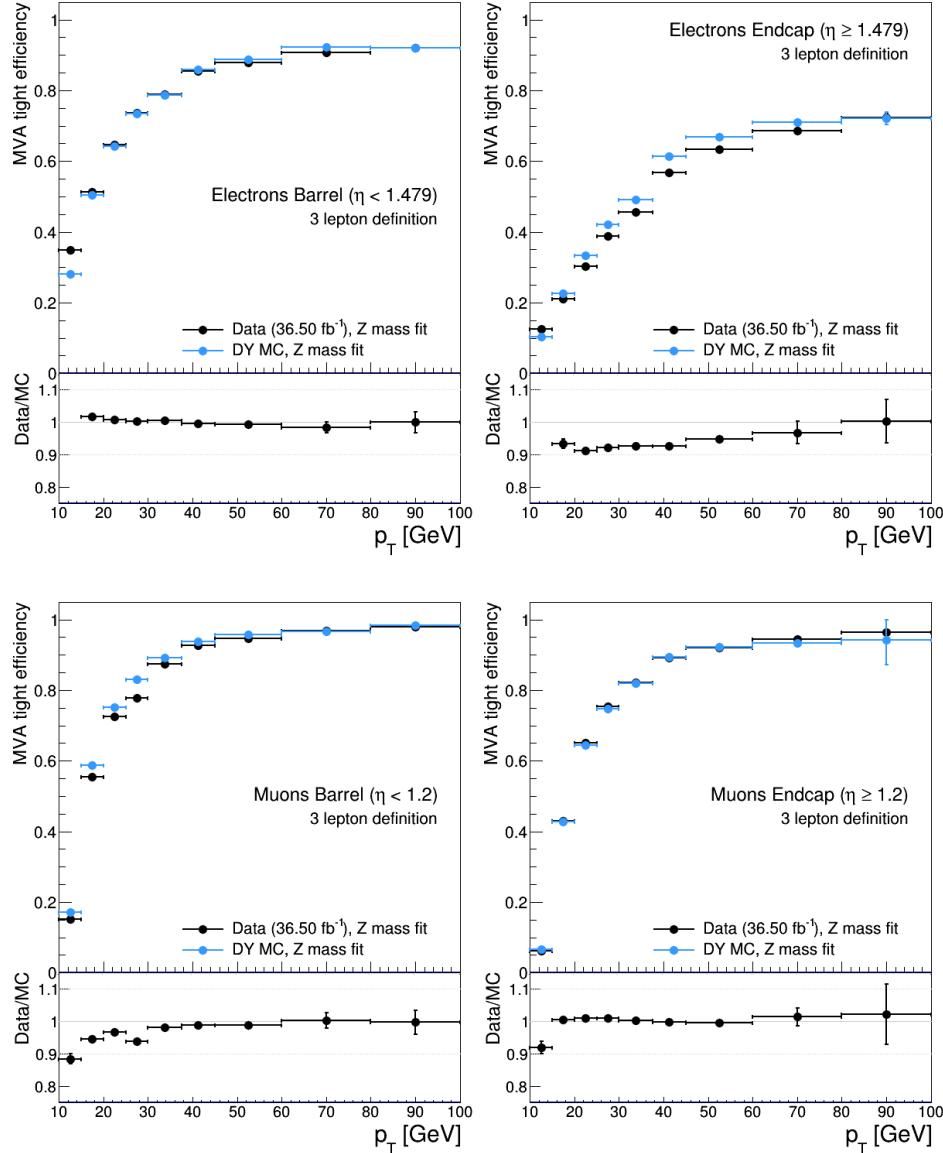
**Figure 6.8:** Tight vs loose selection efficiencies for electrons (top), and muons (bottom), for the  $2lss$  definition, i.e., including the tight-charge requirement.

2677        Efficiencies of reconstruction and selecting loose leptons are measured both for  
 2678        muons and electrons using a tag and probe method on both data and MC, using  
 2679         $Z \rightarrow \ell^+ \ell^-$  [157]. The scale factors are derived from the ratio of efficiencies  $\varepsilon_i(p_T, \eta)$

2680 measured for a given lepton in data/MC, according to

$$\rho(p_T, \eta) = \frac{\varepsilon_{data}(p_T, \eta)}{\varepsilon_{MC}(p_T, \eta)}. \quad (6.5)$$

2681 The scale factor for each event is used to correct the weight of the event in the



**Figure 6.9:** Tight vs loose selection efficiencies for electrons (top), and muons (bottom), for the  $3l$  channel not including the tight-charge requirement.

2682 full sample; therefore, the full simulation correction is given by the product of all  
 2683 the individual scale factors. The scale factors used in this thesis are inherited from  
 2684 Reference [149] which in turns inherited them from leptonic SUSY analyses using  
 2685 equivalent lepton selections.

2686 The efficiency of applying the tight selection as defined in Tables 6.4 and 6.5, on  
 2687 the loose leptons is determined by using a tag and probe method on a sample of Drell-  
 2688 Yan enriched events. Figures 6.8 and 6.9 show the efficiencies for the  $2lss$  channel and  
 2689  $3l$  channel respectively. Efficiencies in the  $2lss$  channel have been produced including  
 2690 the tight-charge requirement, while for the  $3l$  channel it is not included. Number  
 2691 of passed and failed probes are determined from a fit to the invariant mass of the  
 2692 dilepton system. Simulation is corrected using these scale factors; note that they  
 2693 depend on  $\eta$  and  $p_T$ .

### 2694 **6.5.3 Jets and $b$ -jet tagging**

2695 In this analysis, jets are reconstructed by clustering PF candidates using the anti- $k_t$   
 2696 algorithm with parameter distance  $\Delta R = 0.4$ ; those charged hadrons that are not  
 2697 consistent with the selected primary vertex are discarded from the clustering. The  
 2698 jet energy is then corrected for the varying response of the detector as a function of  
 2699 transverse momentum  $p_T$  and pseudorapidity  $\eta$ . Jets are selected for being used in the  
 2700 analysis only if they have  $p_T > 25$  GeV and are separated from any selected leptons  
 2701 by  $\Delta R > 0.4$ .

2702 Jets coming from the primary vertex and jets coming from pile-up vertices are  
 2703 distinguished using a MVA discriminator based on the differences in the jet shapes,  
 2704 in the relative multiplicity of charged and neutral components, and in the different  
 2705 fraction of transverse momentum which is carried by the most energetic components.

2706 Jet tracks are also required to be compatible with the primary vertex.

2707 Jets originated from the hadronization of a  $b$  quark are selected using a MVA  
 2708 likelihood discriminant which uses track-based lifetime information and reconstructed  
 2709 secondary vertices (CSV algorithm). Only jets within the CMS tracker acceptance  
 2710 ( $\eta < 2.4$ ) are identified with this tool. Data samples are used to measure the efficiency  
 2711 of the  $b$ -jet tagging and the probability to misidentify jets from light quarks or gluons;  
 2712 in both cases the measurements are parametrized as a function of the jet  $p_T$  and  $\eta$   
 2713 and later used to correct differences between the data and MC simulation in the  $b$   
 2714 tagging performance, by applying per-jet weights to the simulation, dependent on  
 2715 the jet  $p_T$ ,  $\eta$ ,  $b$  tagging discriminator, and flavor (from the MC generation/simulation  
 2716 truth information) [151]. The per-event weight is taken as the product of the per-jet  
 2717 weights, including those of the jets associated to the leptons. The weights are derived  
 2718 on  $t\bar{t}$  and Z+jets events.

2719 Two working points are defined, based on the CSV algorithm output: *loose* work-  
 2720 ing point ( $\text{CSV} > 0.46$ ) with a  $b$  signal tagging efficiency of about 83%, and *medium*  
 2721 working point ( $\text{CSV} > 0.80$ ) with  $b$ -tagging efficiency of about 69% [152]. Tagging of  
 2722 jets from charm quarks have efficiencies of about 40% and 18% for loose and medium  
 2723 working points respectively. Separate scale factors are applied to jets originating from  
 2724 bottom/charm quarks and from light quarks in simulated events to match the tagging  
 2725 efficiencies measured in the data.

#### 2726 6.5.4 Missing Energy MET

2727 As stated in Section 3.4.1, the MET vector is calculated as the negative of the vector  
 2728 sum of transverse momenta of all PF candidates in the event and its magnitude is  
 2729 referred to as  $E_T^{\text{miss}}$ . Due to pile-up interactions, the performance in determining

2730 MET is degraded; in order to correct for that, the energy from the selected jets and  
 2731 leptons that compose the event is assigned to the variable  $H_T^{miss}$ . It is calculated in  
 2732 the same way as  $E_T^{miss}$  and although it has worse resolution than  $E_T^{miss}$ , it is more  
 2733 robust in the sense that it does not rely on the soft part of the event. The event  
 2734 selection uses a linear discriminator based on the two variables given by

$$E_T^{miss, LD} = 0.00397 * E_T^{miss} + 0.00265 * H_T^{miss} \quad (6.6)$$

2735 taking advantage of the fact that the correlation between  $E_T^{miss}$  and  $H_T^{miss}$  is less  
 2736 for events with instrumental missing energy than for events with real missing energy.  
 2737 The working point  $E_T^{miss, LD} > 0.2$  was chosen to ensure a good signal efficiency while  
 2738 keeping an efficient background rejection.

## 2739 6.6 Event selection

2740 Events are selected considering the features of the signal process and the decay sig-  
 2741 nature as described in Section 6.2. At the trigger level, events are selected to contain  
 2742 either one, two, or three leptons with minimal  $p_T$  thresholds:

- 2743 • single-lepton trigger → 24 GeV for muons and at 27 GeV for electrons
- 2744 • double-lepton triggers → leading and sub-leading leptons: 17 and 8 GeV for  
 2745 muons and 23 and 12 GeV for electrons.
- 2746 • three-lepton triggers → threshold on the third hardest lepton in the event: 5  
 2747 and 9 GeV for muons and electrons, respectively.

2748 The offline event selection level targets the specific topology of the  $tHq$  signal  
 2749 with  $H \rightarrow WW$  and  $t \rightarrow Wb \rightarrow l\nu b$ ; therefore, the resulting state is composed of three

2750 W bosons, one  $b$  quark, and a light spectator quark at high rapidity. The selection  
 2751 criteria for the two channels exploited in this analysis are summarized in Table 6.6.  
 2752 This selection includes contributions from  $H \rightarrow \tau\tau$  and  $H \rightarrow ZZ$  as well.

<b>Same-sign <math>\ell\ell</math> channel <math>e^\pm\mu^\pm, \mu^\pm\mu^\pm</math></b>	<b><math>\ell\ell\ell</math> channel</b>
Have fired one of the corresponding trigger paths	
No loose leptons with $m_{\ell\ell} < 12\text{GeV}$	
One or more $b$ tagged jets (CSV medium) $ \eta  < 2.4$	
One or more non-tagged jets: central $\rightarrow p_T > 25\text{ GeV}, \eta < 2.4$	
	forward $\rightarrow p_T > 40\text{ GeV}, \eta > 2.4$
$E_T^{miss}_{LD} > 0.2$	
Exactly two tight same-sign leptons	Exactly three tight leptons
Lepton $p_T > 25/15\text{GeV}$	Lepton $p_T > 25/15/15\text{GeV}$
Electrons are triple-charge consistent.	No OSSF lepton pair with $ m_{\ell\ell} - m_Z  < 15\text{GeV}$
Muon $p_T$ resolution: $\Delta p_T/p_T < 0.2$ .	
No ee pair with $ m_{ee} - m_Z  < 10\text{GeV}$	

**Table 6.6:** Summary of event pre-selection.

2753 In the  $2lss$  channel, events with additional tight leptons are vetoed as well as those  
 2754 for which a loose lepton pair has an invariant mass below 12 GeV. A threshold in  $p_T$  of  
 2755 the leading and sub-leading leptons is also required. Events where the two electrons  
 2756 have invariant mass within 10 GeV of the Z boson mass ( $Z$ -veto) are discarded in  
 2757 order to reject events from DY+jets production with charge misidentified electrons.  
 2758 In addition, contribution from the associated production of two W bosons of equal  
 2759 charge and two light jets  $W^\pm W^\pm qq$  and from same-sign W boson pairs can also be  
 2760 produced in double parton scattering (DPS) processes, where each of the colliding  
 2761 protons gives two partons, resulting in two hard interactions.

2762 In the  $3l$  lepton channel, leptons are required to have respectively  $p_T > 25\text{GeV}, >$   
 2763  $> 15\text{ GeV}$ , and  $> 15\text{ GeV}$ . Events with an opposite-sign same-flavor lepton combination  
 2764 (OSSF) with invariant mass within 15 GeV of the Z boson mass are discarded in order  
 2765 to reject events from  $WZ + \text{jets}$  production.

## 2766 6.7 Background modeling and predictions

2767 The dominant background contribution is expected to arise from top quark produc-  
 2768 tion processes, either  $t\bar{t}$  pair production or in  $t\bar{t}$  associated production with a W/Z.  
 2769 Processes with production of single top quarks also contribute, mainly in the associ-  
 2770 ated production with a Z boson ( $tZq$ ) or when produced with both a W and a Z boson  
 2771 ( $tZW$ ). Background contamination from diboson processes is strongly suppressed by  
 2772 imposing the Z-veto, vetoing additional leptons and requiring  $b$ -jets in the event.

2773 The selection criteria in Table 6.6 represent a relatively loose selection that allows  
 2774 to maintain a large signal efficiency while suppressing the main backgrounds; thus  
 2775 that selection is called *pre-selection*. The events obtained from the pre-selection are  
 2776 then used to extract the signal contribution in a second analysis step, using BDT dis-  
 2777 criminators against the main backgrounds of  $t\bar{t}W/t\bar{t}Z$  and non-prompt leptons from  
 2778  $t\bar{t}$ . The shape of the discriminator variables is then fit to the observed data distribu-  
 2779 tion to estimate the signal and background yields, simultaneously for all channels.

2780 Irreducible backgrounds are reliably estimated from MC simulated events; there-  
 2781 fore, in this analysis all backgrounds involving prompt leptons are estimated in this  
 2782 way. Reducible backgrounds, like non-prompt lepton backgrounds, are not well pre-  
 2783 dicted by simulation, hence, they are estimated using data-driven methods.

### 2784 6.7.1 $t\bar{t}V$ and diboson backgrounds

2785 Backgrounds from  $t\bar{t}W$  and  $t\bar{t}Z$  processes are estimated using simulated events, cor-  
 2786 rected for data/MC differences and inefficiencies (trigger and lepton selection) in the  
 2787 same way as signal events. Their production cross sections are calculated at NLO of  
 2788 QCD and EWK, considering theoretical uncertainties from unknown higher orders of  
 2789 12% for  $t\bar{t}W$  and 10% for  $t\bar{t}Z$ . Additional uncertainties arise from the knowledge of

2790 PDFs and  $\alpha_s$  of about 4% each for  $t\bar{t}W$  and  $t\bar{t}Z$ .

2791 The diboson contribution is also estimated from simulated events; however, the  
 2792 overall normalization of this process is obtained from a dedicated control region.  
 2793 The motivation behind that strategy is that even though the measured inclusive  
 2794 cross section for diboson processes ( $WZ, ZZ$ ) is in good agreement with the NLO  
 2795 calculations [149], that agreement is perturbed when leptonic  $Z$  decays and hadronic  
 2796 jets in the final state are required; those requirements are precisely the ones that  
 2797 make the diboson production a background for the  $tHq$  signal. Thus, by using a  
 2798 dedicated control region dominated by  $WZ$  production<sup>4</sup>, the overall normalization is  
 2799 constrained.

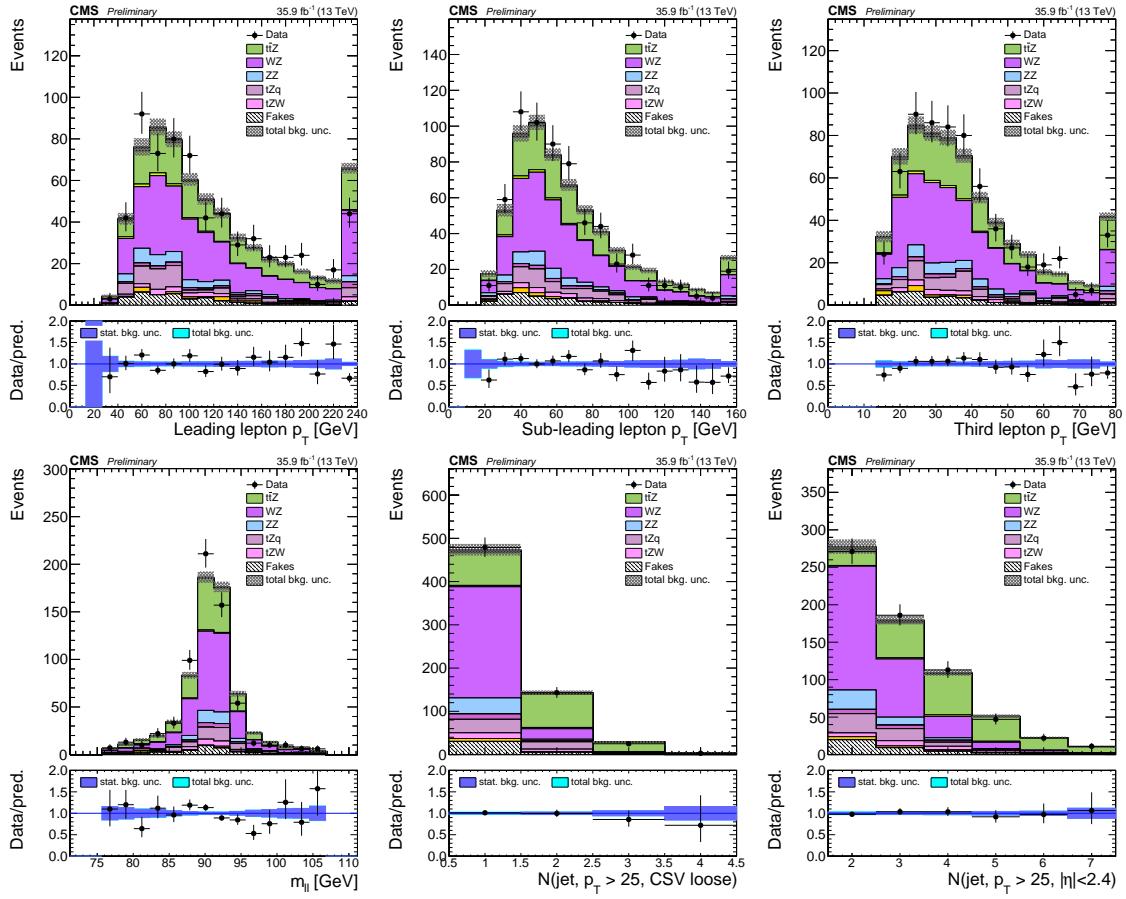
2800 The control region is defined by the presence of at least three leptons, of which  
 2801 one opposite-sign pair must be compatible with a  $Z$  boson decay, i.e., invert the  $Z$ -  
 2802 veto which makes the control region orthogonal to signal region; the b-jet tagging  
 2803 requirements is also inverted with respect to the signal region, i.e., require two not  
 2804 b-jets. A scale factor is extracted from the predicted distribution of  $WZ$  events in the  
 2805 control region, and the observed data, while keeping other processes fixed; this factor  
 2806 is used to scale the diboson prediction in the signal selection region. More details  
 2807 about the procedure used can be found in Reference [149] from where the scale factor  
 2808 is taken.

2809 In order to test the usability of the diboson background scale factor in this analysis,  
 2810 a  $Z$ -enriched control region<sup>5</sup> was defined by inverting the  $Z$ -veto and requiring exactly  
 2811 three tight leptons with  $p_T > 25/15/15$  GeV, one or more jets passing the CSVv2 loose  
 2812 working point and less than four central jets. Figure 6.10 shows the distribution of  
 2813 three variables in the diboson control region; the good agreement between MC and

---

<sup>4</sup>  $ZZ$  background is strongly reduced by the cut on MET.

<sup>5</sup> This control region is different to the one used to find the scale factor.



**Figure 6.10:** Kinematic distributions in the diboson control region.

2814 data motivates the adoption of the diboson background scale factor.

2815 Most of the diboson events passing the signal selection contain jets from light  
 2816 quarks and gluons that are incorrectly tagged as  $b$ -jets; it makes the estimate mainly  
 2817 sensitive to the experimental uncertainty in the mis-tag rate rather than the theore-  
 2818 tical uncertainty in the jet flavor composition. The overall uncertainty assigned to  
 2819 the diboson prediction is estimated from the statistical uncertainty due to the limited  
 2820 sample size in the control region (30%), the residual background in the control region  
 2821 (20%), the uncertainties on the  $b$ -tagging rate (10-40%), and from the knowledge of  
 2822 PDFs and the theoretical uncertainties of the extrapolation (up to 10%).

2823 **6.7.2 Non-prompt and charge mis-ID backgrounds**

2824 The non-prompt lepton background contribution to the final selection is estimated  
 2825 using the fake factor method. The main idea of the method is to define a control  
 2826 region of events enriched in the background to estimate and determine a factor that  
 2827 relates (extrapolates) these events to those in the signal region. The method is data-  
 2828 driven in the sense that the control sample is selected from data, and the extrapolation  
 2829 factor is measured from data.

2830 In the signal region of this analysis, non-prompt leptons are predominantly pro-  
 2831 duced in  $t\bar{t}$  events, with a much smaller contribution, from Drell-Yan production;  
 2832 therefore, the control region also known as *application region*, is defined by modifying  
 2833 the event selection criteria in such a way that most of the events after selection are  
 2834  $t\bar{t}$  events and thus the misidentification rate is increased. The application regions  
 2835 for electrons and muons are defined by the *fakeable* object definitions in Tables 6.4  
 2836 and 6.5. Since the fakeable definition is a loosened version of the tight definition, in  
 2837 the context of fake rates, the fakeable definition becomes the loose selection.

2838 The ratio between the number of events that pass both, the loose and tight se-  
 2839 lections, and the number of events that pass the loose selection but fail the tight  
 2840 one, corresponds to the *loose-to-tight ratio or fake factor/rate (f)*. The measurement  
 2841 of the fake factor is made using two background dominated data samples, collected  
 2842 with dedicated triggers, as a function of  $p_T$  and  $|\eta|$  and separately for muons and  
 2843 electrons:

- 2844 • A sample dominated by QCD multijet events, collected using single lepton trig-  
 2845 gers at relatively high  $p_T$  thresholds. It is used to extract ratios for lepton  
 2846 candidates with  $p_T$  above 30 GeV.
- 2847 • A sample dominated by Z + jets events, where the two high  $p_T$  leptons resulting

2848 from the Z decay are used to trigger the events without biasing the  $p_T$  spectrum  
 2849 of a third lepton at low transverse momentum. It is used to determine the ratios  
 2850 for low  $p_T$  leptons.

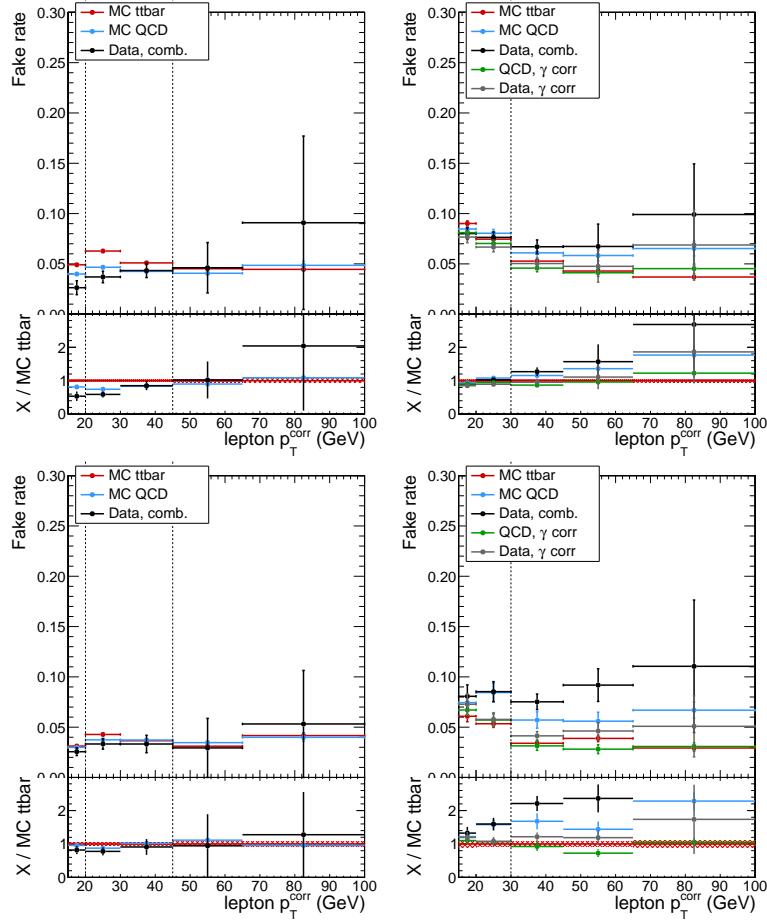
2851 Processes like  $W + \text{jets}$ ,  $Z + \text{jets}$ ,  $WZ$  and  $ZZ$  produce prompt leptons that  
 2852 contaminate the samples; thus, they are suppressed by vetoing additional leptons in  
 2853 the selection, and the residual contamination is then subtracted using the transverse  
 2854 mass as a discriminating variable.

2855 The extrapolation from the application region to the signal region is performed  
 2856 by weighting the events in the application region using the fake factor according to  
 2857 the following rules:

- 2858     • events with one lepton failing the tight criteria are weighted with the factor  
     2859      $\frac{f}{(1-f)}$  for the estimate to the signal region.
- 2860     • events with two leptons (i,j) failing the tight criteria are weighted with the factor  
     2861      $-\frac{f_i f_j}{(1-f_i)(1-f_j)}$  for the estimate to the signal region.
- 2862     • events with three leptons (i,j,k) failing the tight criteria are weighted with the  
     2863     factor  $\frac{f_i f_j f_k}{(1-f_i)(1-f_j)(1-f_k)}$  for the estimate to the signal region.

2864 Figure 6.11 shows the fake rates for electrons and muons used in this analysis  
 2865 which were taken from the studies in Reference [149].

2866 The resulting prediction of the event yield in the signal selection carries an uncer-  
 2867 tainty of 30-50% which is composed of the statistical uncertainty in the measurement  
 2868 of the fake rates due to prescaling of lepton triggers, the uncertainty in the subtraction  
 2869 of residual prompt leptons from the control region, and from testing the closure of the  
 2870 method in simulated background events; hence, it is one of the dominant limitations  
 2871 on the performance of multilepton analyses in general and this analysis in particular.



**Figure 6.11:** Fake rate measurement in events in data for muons (left column) and electrons (right column). Predictions from simulated events in the measurement region (blue) and from non-prompt leptons in  $t\bar{t}$  (red) are included for comparison. Top row is for  $|\eta| < 2.5$  and bottom row for  $|\eta| > 2.5$ .

Finally, an additional source of background arises in the  $2lss$  channel from events with an originally opposite-sign lepton pair for which the charge of one of the leptons is misidentified (*charge mis-ID*); usually this happens because of the conversion of hard bremsstrahlung photons emitted from the initial lepton, hence, it is more likely to happen for electrons than for muons.

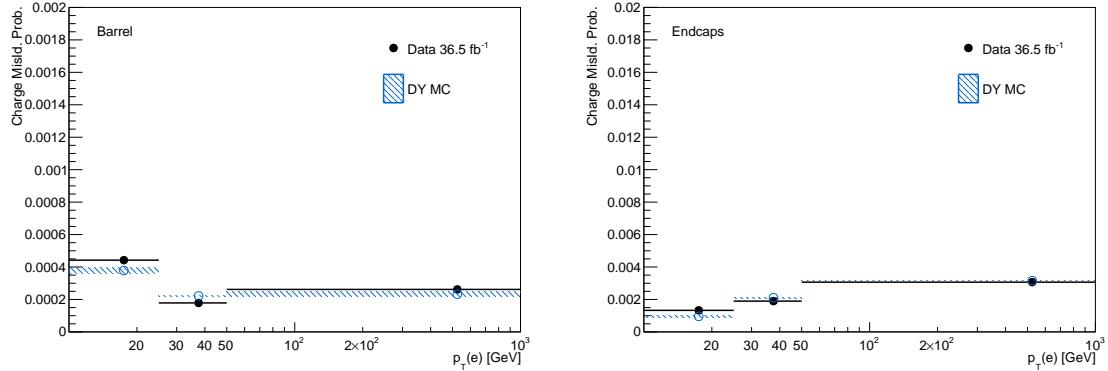
The charge mis-ID background is estimated from the yield of opposite-sign event in the signal region by measuring the charge mis-ID probability in same-sign and opposite-sign events compatible with a Z boson decay, in several bins of  $p_T$  and  $\eta$ ,

2880 and weighting events with opposite-sign leptons in the signal selection.

Data	$10 \leq p_T < 25$ GeV	$25 \leq p_T < 50$ GeV	$50 \text{ GeV} \leq p_T$
$0 \leq \eta < 1.48$	$0.0442 \pm 0.0011$	$0.0179 \pm 0.0004$	$0.0262 \pm 0.0020$
$1.48 \leq \eta < 2.5$	$0.1329 \pm 0.0066$	$0.1898 \pm 0.0014$	$0.3067 \pm 0.0113$
MC			
$0 \leq \eta < 1.48$	$0.0378 \pm 0.0016$	$0.0222 \pm 0.0003$	$0.0233 \pm 0.0015$
$1.48 \leq \eta < 2.5$	$0.0956 \pm 0.0044$	$0.2108 \pm 0.0027$	$0.3157 \pm 0.0018$

**Table 6.7:** Electron charge mis-ID probabilities (in percent), determined in data (top) and Drell-Yan MC (bottom) [149].

2881 The charge mis-ID probability is found to be negligible for this analysis for muons,  
 2882 whereas for electrons it ranges from about 0.02% in the barrel section ( $|\eta| < 1.48$ )  
 2883 up to about 0.35% in the detector endcaps ( $1.48 < |\eta| < 2.5$ ). as shown in Table 6.7  
 2884 and Figure 6.12.



**Figure 6.12:** Electron charge mis-ID probabilities as a function of  $p_T$  for  $|\eta| < 2.5$  (left)  
 and  $|\eta| < 2.5$  (right) [149].

2885 The contribution from charge mis-ID electrons in signal selection of this analysis  
 2886 comes mainly from  $t\bar{t}$  and Drell-Yan events. The systematic uncertainty of the nor-  
 2887 malization of the charge mis-ID estimate is evaluated at about 30%, arising from a  
 2888 slight disagreement of the mis-ID probability between data and simulation. Given  
 2889 that it only affects the  $e\mu$  channel, its impact on the final sensitivity is very limited.

## 2890 6.8 Pre-selection yields

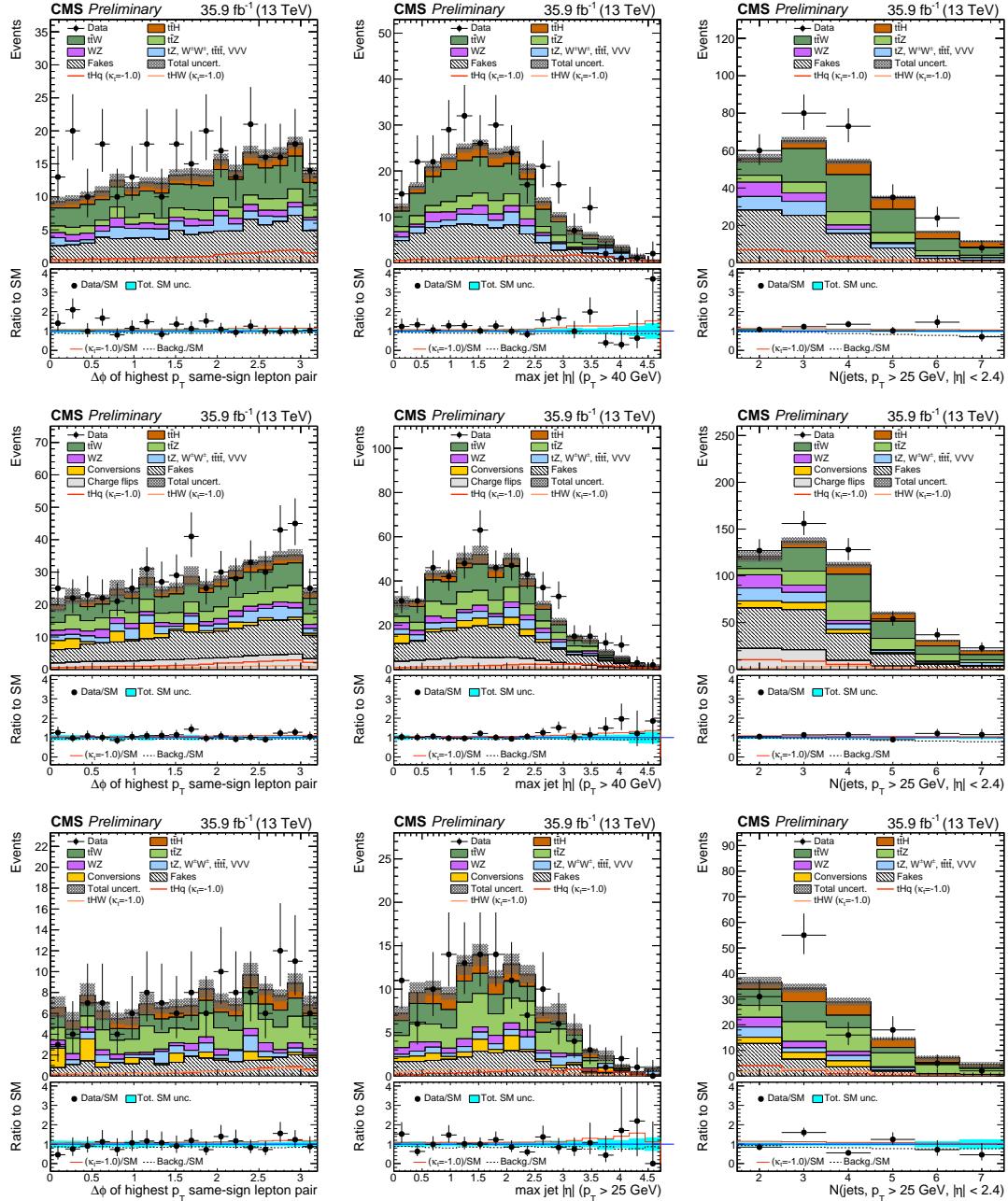
2891 The expected and observed event yields of the pre-selection are shown in Table 6.8;  
 2892 Figure 6.13 shows the distributions of some relevant kinematic variables, normalized  
 2893 to the cross section of the respective processes and to the integrated luminosity. The  
 2894 remaining variables distributions are shown in Appendix B.1.

	$3\ell$	$\mu^\pm \mu^\pm$	$e^\pm \mu^\pm$
$t\bar{t}W$	$22.50 \pm 0.35$	$68.03 \pm 0.61$	$97.00 \pm 0.71$
$t\bar{t}Z/\gamma^*$	$32.80 \pm 1.79$	$25.89 \pm 1.12$	$64.82 \pm 2.42$
$WZ$	$8.22 \pm 0.86$	$15.07 \pm 1.19$	$26.25 \pm 1.57$
$ZZ$	$1.62 \pm 0.33$	$1.16 \pm 0.29$	$2.86 \pm 0.45$
$W^\pm W^\pm qq$	–	$3.96 \pm 0.52$	$6.99 \pm 0.69$
$W^\pm W^\pm(\text{DPS})$	–	$2.48 \pm 0.42$	$4.17 \pm 0.54$
VVV	$0.42 \pm 0.16$	$2.99 \pm 0.34$	$4.85 \pm 0.43$
ttt	$1.84 \pm 0.44$	$2.32 \pm 0.45$	$4.06 \pm 0.57$
tZq	$3.92 \pm 1.48$	$5.77 \pm 2.24$	$10.73 \pm 3.03$
tZW	$1.70 \pm 0.12$	$2.13 \pm 0.13$	$3.91 \pm 0.18$
$\gamma$ conversions	$7.43 \pm 1.94$	–	$23.81 \pm 6.04$
Non-prompt	$25.61 \pm 1.26$	$80.94 \pm 2.02$	$135.34 \pm 2.83$
Charge mis-ID	–	–	$58.50 \pm 0.31$
All backgrounds	$106.05 \pm 3.45$	$210.74 \pm 3.61$	$443.30 \pm 8.01$
$tHq$ ( $\kappa_t = -1.0$ )	$7.48 \pm 0.14$	$18.48 \pm 0.22$	$27.41 \pm 0.27$
$tHW$ ( $\kappa_V = -1.0$ )	$7.38 \pm 0.16$	$7.72 \pm 0.17$	$11.23 \pm 0.20$
$t\bar{t}H$	$18.29 \pm 0.41$	$24.18 \pm 0.48$	$35.21 \pm 0.58$
Data ( $35.9 fb^{-1}$ )	127	280	525

**Table 6.8:** Expected and observed yields for  $35.9 fb^{-1}$  after the pre-selection in all final states. Uncertainties are statistical only.

2895 For the  $tH$  and  $t\bar{t}H$  processes, the largest contribution comes from Higgs decays  
 2896 to WW (about 75%), followed by  $\tau\tau$  (about 20%) and ZZ (about 5%). Other Higgs  
 2897 production modes contribute negligible event yields (< 5% of the  $tH + t\bar{t}H$  yield) as  
 2898 shown in Table 6.9.

2899 A significant fraction of selected data events (about 50% in the dilepton channels,  
 2900 and about 80% in the trilepton channel) also passes the selection used in the dedicated



**Figure 6.13:** Distributions of discriminating variables for the event pre-selection for the same-sign  $\mu^\pm\mu^\pm$  channel (top row), the same-sign  $e^\pm\mu^\pm$  channel (middle row) and three lepton channel (bottom row), normalized to  $35.9 \text{ fb}^{-1}$ , before fitting the signal discriminant to the observed data. Uncertainties are statistical and unconstrained (pre-fit) normalization systematics. The shape of the two  $tH$  signals for  $\kappa_t = -1.0$  is shown, normalized to their respective cross sections for  $\kappa_t = -1.0, \kappa_V = 1.0$ .

	$3\ell$	$\mu^\pm \mu^\pm$	
$tHq$ (Inclusive)	<b>6.57</b>	100.0%	<b>17.38</b> 100.0%
$tHq(H \rightarrow WW)$	4.84	73.9%	13.33 76.9%
$tHq(H \rightarrow \tau\tau)$	1.04	15.9%	3.62 20.6%
$tHq(H \rightarrow ZZ)$	0.48	7.2%	0.37 2.2%
$tHq(H \rightarrow \mu\mu)$	0.21	3.0%	0.04 0.2%
$tHq(H \rightarrow \gamma\gamma)$	< 0.01	0.1%	0.02 0.1%
$tHq(H \rightarrow bb)$	< 0.01	< 0.1%	0.01 < 0.1%
$tHW$ (Inclusive)	<b>7.32</b>	100.0%	<b>7.62</b> 100.0%
$tHW(H \rightarrow WW)$	5.50	76.9%	5.60 74.1%
$tHW(H \rightarrow \tau\tau)$	1.40	20.6%	1.81 23.1%
$tHW(H \rightarrow ZZ)$	0.31	2.2%	0.21 2.7%
$tHW(H \rightarrow \mu\mu)$	0.12	0.2%	0.01 0.1%
$tHW(H \rightarrow \gamma\gamma)$	< 0.01	< 0.1%	< 0.01 < 0.1%
$tHW(H \rightarrow bb)$	< 0.01	< 0.1%	< 0.01 < 0.1%

**Table 6.9:** Signal yields split by decay channels of the Higgs boson. Forward jet  $p_T$  cut at 25 GeV.

2901 search for  $tH$  in multilepton channels [149]. This is particularly important when  
 2902 considering a possible combination of the measurements from both studies. More  
 2903 details about the overlap between these two analyses are presented in Appendix E.

## 2904 6.9 Signal discrimination

2905 The production cross section for the signal processes  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  is only  
 2906 about 600 fb (the enhancement provided by inverted couplings,  $\kappa_t = -1$  almost double  
 2907 it), resulting in a small signal to background ratio even for a tight selection. A  
 2908 multivariate method is hence employed to train discriminators to separate  $tH$  signal  
 2909 events from the dominant background events.

2910 **6.9.1 MVA classifiers evaluation**

2911 Several MVA classifier algorithms were evaluated in order to determine the most  
 2912 appropriate method for this analysis<sup>6</sup>. The comparison is based on the performance  
 2913 of the classifiers, encoded in the plot of the background rejection as a function of the  
 2914 signal efficiency (ROC curve). The top row of Figure 6.14 shows the ROC curves for  
 2915 evaluated methods; two separated training were performed in the  $3l$  channel: against  
 2916  $t\bar{t}$  (right) and  $t\bar{t}V$  (left) processes.

2917 In both cases, the gradient boosted decision tree *BDTG* (*BDTA\_GRAD* in the  
 2918 plot) classifier offers the best results, followed by the adaptive BDT classifier (*BDTA*);  
 2919 the several Fisher classifiers tested, which differ in their parameters and/or boosting  
 2920 method, they offer similar performance among them, while the k-Nearest Neighbour  
 2921 (kNN) classifier performance is below the rest of the classifiers. The corresponding  
 2922 ROC curves and in the  $2lss$  channel for trainings against  $t\bar{t}V$ (left) and  $t\bar{t}$  (right)  
 2923 processes are shown in the bottom row of Figure 6.14; the BDTG performance is  
 2924 similar to that in the  $3l$  channel.

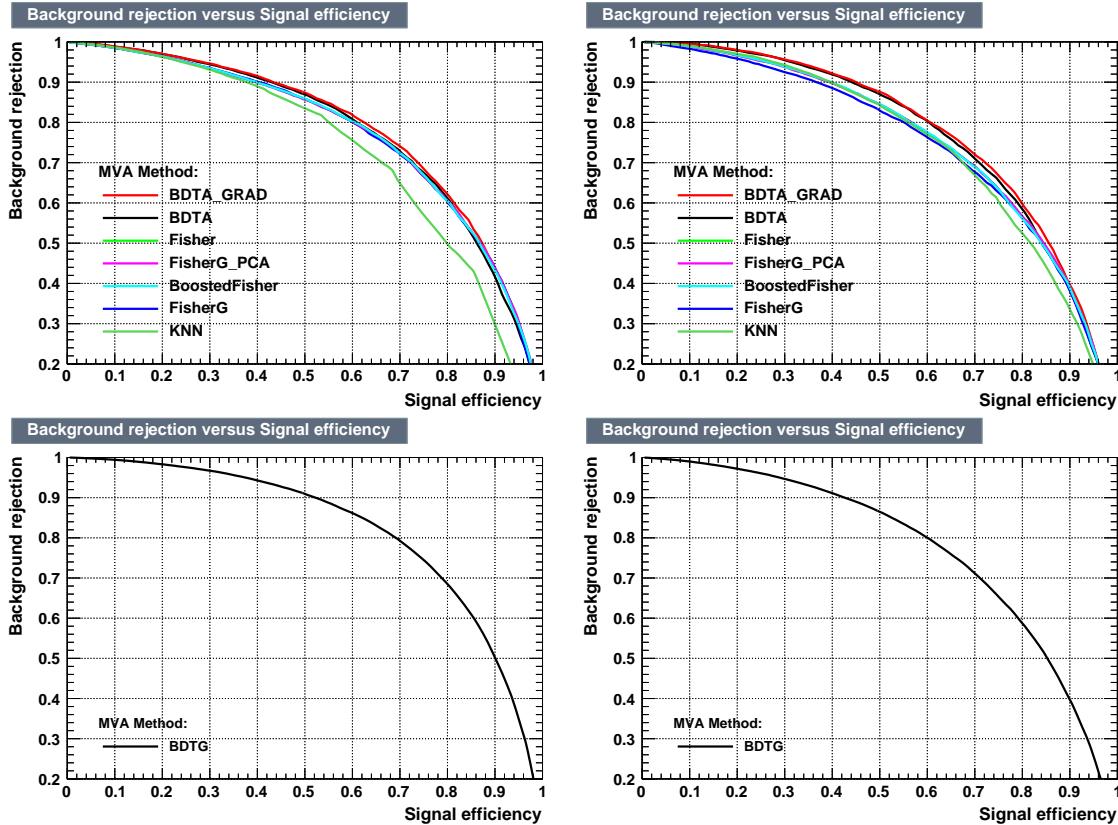
2925 **6.9.2 Discriminating variables**

2926 The classifier chosen to separate the  $tHq$  signal from the main backgrounds is the  
 2927 *BDTG* classifier, trained on simulated signal and background events. The samples  
 2928 used in the training are the  $tHq$  sample in Table 6.2, the samples in the third section  
 2929 of Table A.4 and the samples marked with an \* in the same table.

2930 As explained in Section 5.1.1, a set of discriminating variables are given as input to  
 2931 the *BDTG* which combines the individual discrimination power of each input variable

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<sup>6</sup> The choice of the tested algorithms was based on the recommendations provided by the official TMVA user guide, the experience from previous analyses and considering the expertise of the members of the  $tHq$  and  $t\bar{t}H$  analyses groups. Only the BDT classifier is described in this thesis and a detailed description of all available methods can be found in Reference [127]



**Figure 6.14:** Top: Background rejection vs signal efficiency (ROC curves) for various MVA classifiers in the  $3l$  channel for training against  $t\bar{t}V$  (left) and  $t\bar{t}$  (right). Bottom: background rejection vs signal efficiency (ROC curve) in the  $2lss$  channel for a single discriminator: BDTG, against  $t\bar{t}V$  (left) and  $t\bar{t}$  (right).

2932 to produce a discriminator with the maximum discrimination power. Table 6.10 lists  
 2933 the input variables used in the BDTG trainings for this analysis. The same set of  
 2934 input variables was used to produce the plots for MVA classifiers evaluation.

2935 Plots in Figure 6.15 shows the BDTG input variables distributions for the signal  
 2936 and background samples, in the  $3l$  channels.

2937 All the input variables have some discrimination power, however, that power is  
 2938 bigger for some of them; for instance, the third lepton  $p_T$  plot (top left in Figure 6.15)  
 2939 shows some discrimination power against WZ and VVV backgrounds for which there  
 2940 is a peak around 30 GeV while  $tHq$  peak around 18 GeV; although the discrimination

Variable name	Description
nJet25	Number of jets with $p_T > 25$ GeV, $ \eta  < 2.4$
nJetEta1	Number of jets with $ \eta  > 1.0$ , non-CSV-loose
MaxEtaJet25	Max. $ \eta $ of any (non-CSV-loose) jet with $p_T > 25$ GeV
deltaFwdJetClosestLep	$\Delta\eta$ forward light jet and closest lepton
deltaFwdJetBJet	$\Delta\eta$ forward light jet and hardest CSV loose jet
deltaFwdJet2BJet	$\Delta\eta$ forward light jet and second hardest CSV loose jet
Lep3Pt/Lep2Pt	$p_T$ of the 3 <sup>rd</sup> lepton (2 <sup>nd</sup> for ss2l)
totCharge	Sum of lepton charges
minDRll	Min $\Delta R$ any two leptons
dphiHighestPtSSPair	$\Delta\phi$ of highest $p_T$ same-sign lepton pair

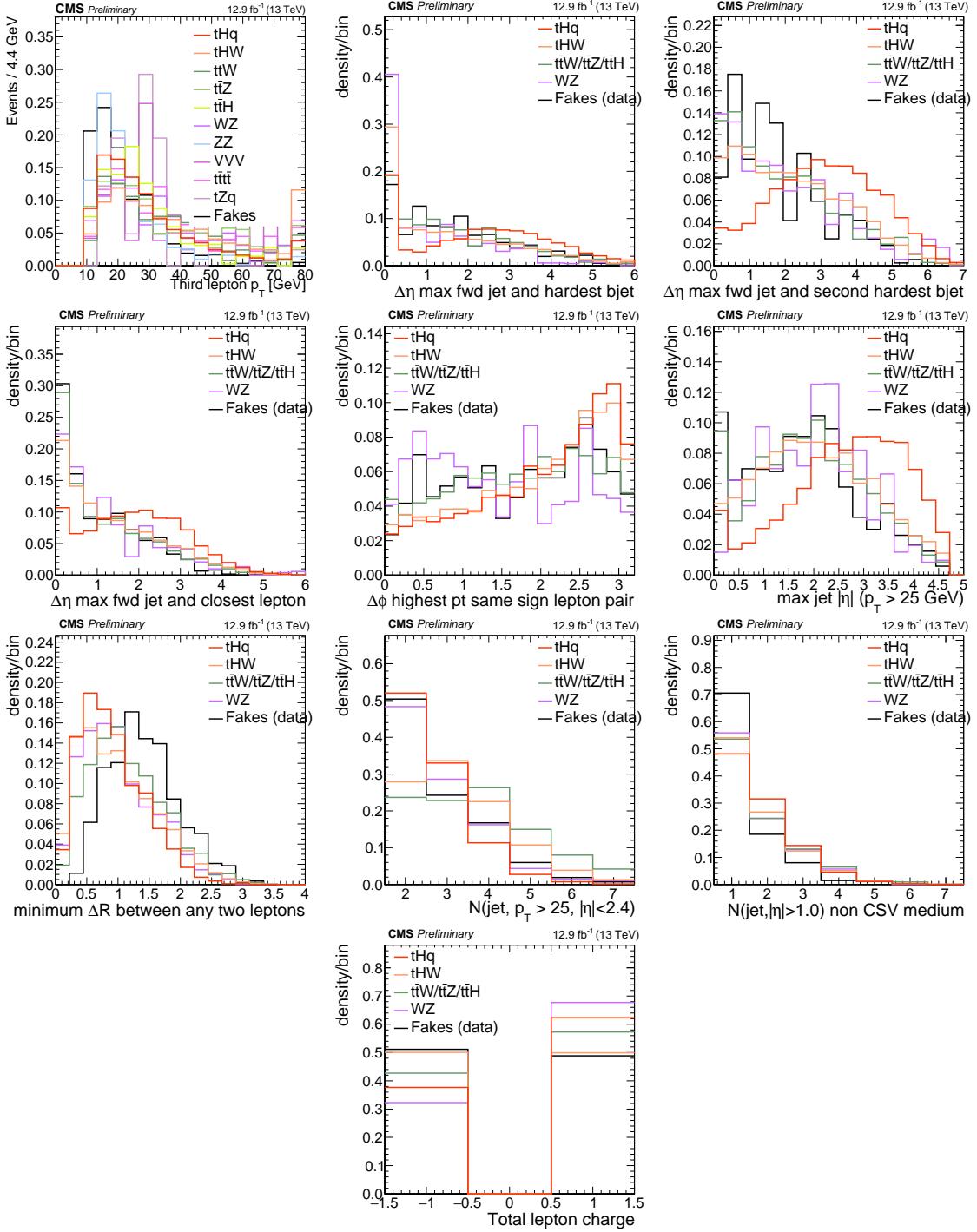
**Table 6.10:** BDTG input variables. First section lists variables related to jet multiplicities; second section lists variables related to forward jet activity, and third section lists variables related to lepton kinematics.

2941 power does not cover all the backgrounds, it counts for the final discriminator. A  
 2942 similar situation can be seen in the plot for the number of jets (row three, column two);  
 2943  $t\bar{t}W$ ,  $t\bar{t}Z$  and  $t\bar{t}H$  processes tend to have more jets compared to the  $tHq$  process. The  
 2944 discrimination power is more evident in other plots like in the plot of the maximum  
 2945  $|\eta|$  of the jets in the event (row two, column three). The same or equivalent input  
 2946 variables are found to be performing well for both  $3l$  and  $2lss$  channels. Figure B.4  
 2947 shows the corresponding input variables distribution plots for the  $2lss$  channel.

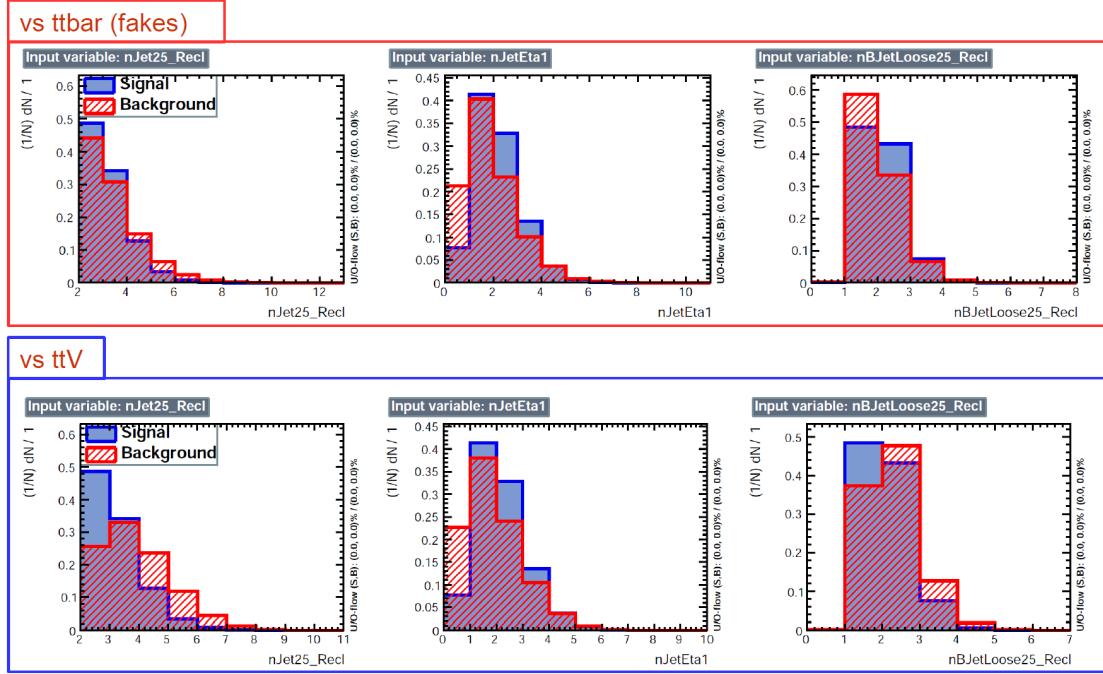
#### 2948 Discrimination power from BDTG classifier

2949 The Discrimination power of the input variables can also be evaluated from the BDTG  
 2950 training, exclusively for the training samples, i.e., dominant backgrounds ( $t\bar{t}$  and  $t\bar{t}V$ );  
 2951 the training samples are submitted to the selection cuts on Table 6.6.

2952 Figure 6.16 shows the comparison between input variables for the two trainings  
 2953 in the  $3l$  channel; it reveals that some variables show opposite behavior for the two  
 2954 background sources, which results in potentially screening the discrimination power  
 2955 if they were to be used in a single discriminant, i.e., if the training would join  $t\bar{t}$  and



**Figure 6.15:** Distributions of the BDTG classifier input variables (not normalized) for signal discrimination in the  $3l$  channel.



**Figure 6.16:** BDT input variables as seen by BDTG classifier for the  $3l$  channel,  $tHq$  signal(blue) discriminated against  $t\bar{t}V$  background (red).

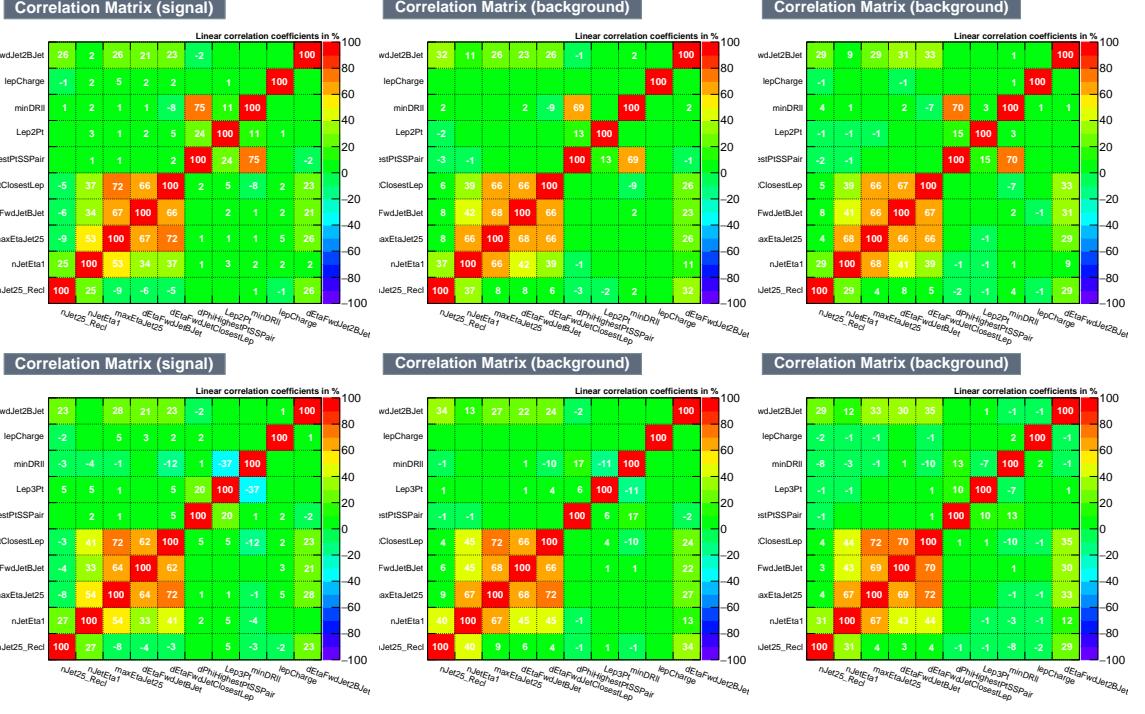
2956  $t\bar{t}V$ . For some other variables the distributions are similar in both background cases.

2957 In contrast to the distributions in Figure 6.15 only the dominant backgrounds are  
2958 included; however, the discrimination power agrees among plots.

2959 Figures in the Appendix B.5, B.6, B.7, and B.8 show the input variables  
2960 distributions for the  $2lss$  and  $3l$  channel as seen by the BDTG classifier.

### 2961 Input variables correlations

2962 From Table 6.10, it is clear that the input variables are correlated to some extent.  
2963 These correlations play an important role for some MVA methods like the Fisher  
2964 discriminant method in which the first step consist of performing a linear transfor-  
2965 mation to an phase space where the correlations between variables are removed. In  
2966 the case of BDT, correlations do not affect the performance. Figure 6.17 shows the



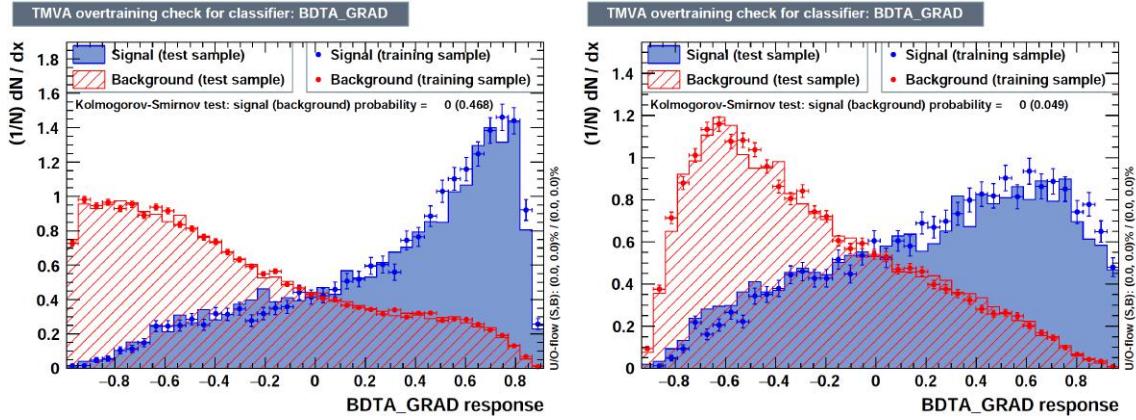
**Figure 6.17:** Signal (left),  $t\bar{t}$  background (middle), and  $t\bar{t}V$  background (right.) correlation matrices for the input variables in the BDTG classifier for the  $2lss$  (top) and  $3l$  (bottom) channels.

2967 linear correlation coefficients for signal and background for the two training cases (the  
 2968 signal values are identical by construction). As expected, strong correlations appears  
 2969 for variables related to the forward jet activity.

### 2970 6.9.3 BDTG classifiers response

2971 After the training stage, the BDTG classifier is tested to ensure its ability to discrim-  
 2972 inate between simulated signal and background events. The BDTG classifier output  
 2973 distributions for signal and backgrounds in the  $3l$  channel are shown in Figure 6.18.  
 2974 As expected, a good discrimination power is obtained using default discriminator  
 2975 parameter values; some overtraining is also visible.

2976 In order to explore further optimization in the BDTG performance, several changes



**Figure 6.18:** BDTG classifier output for trainings against  $t\bar{t}V$ (left) and  $t\bar{t}$  (right). Default BDTG parameters have been used.

from the default BDTG parameters were tested; Table 6.11 list the set of parameters found to be most discriminant with minimal overtraining as shown in Figure 6.19.

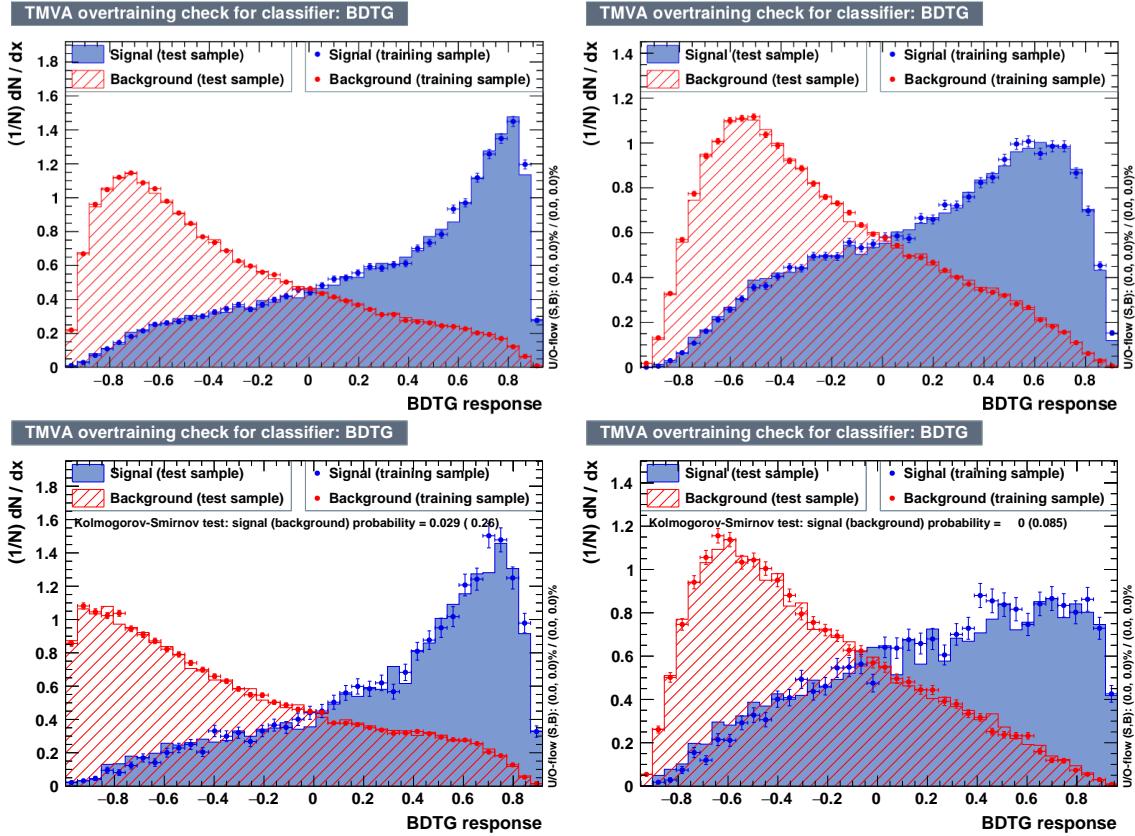
TMVA.Types.kBDT		
Option	Default	Used
NTrees	200	800
BoostType	AdaBoost	Grad
Shrinkage	1	0.1
nCuts	20	50
MaxDepth	3	

**Table 6.11:** Configuration used in the final BDTG training. Parameters not listed were not tested.

The ranking of the input variables by their importance in the classification process is shown in Table 6.12; for both trainings the rankings show almost the same five variables in the first places.

#### 6.9.4 Additional discriminating variables

Given that the forward jet in background processes could be originated from pileup, two additional discriminating variables accounting for that were tested. These additional variables describe the forward jet momentum (`fwdJetPt25`) and the forward



**Figure 6.19:** BDTG classifiers output for training against  $t\bar{t}V$ (left) and  $t\bar{t}$  (right) for  $2lss$  channel(top) and  $3l$  channel (bottom) .

2986 jet identification (fwdJetPUID); their distributions in the  $3l$  channel are shown in  
 2987 Figure 6.20. The forward jet identification distribution shows that for both, signal  
 2988 and background, jets are mostly originated in the primary vertex.

2989 The testing was performed by including in the BDTG input one variable at a  
 2990 time, so the discrimination power of each variable can be evaluated individually, and  
 2991 then both simultaneously. fwdJetPUID was ranked the last place in importance (11)  
 2992 in both training ( $t\bar{t}V$  and  $t\bar{t}$ ) while fwdJetPt25 was ranked 3 in the  $t\bar{t}V$  training and  
 2993 7 in the  $t\bar{t}$  training. When training using 12 variables, fwdJetPt25 was ranked 5 and  
 2994 7 in the  $t\bar{t}V$  and  $t\bar{t}$  trainings respectively, while fwdJetPUID was ranked 12 in both  
 2995 cases.

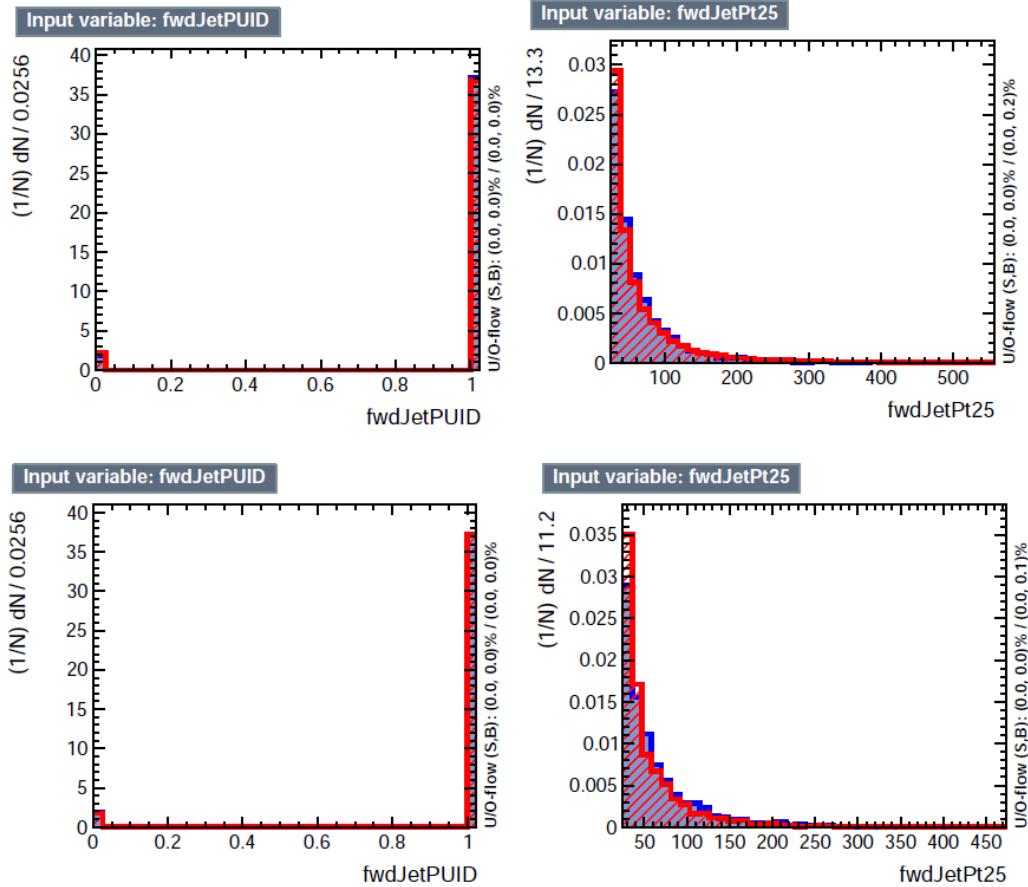
Rank	$t\bar{t}$ training		$t\bar{t}V$ training	
	Variable		Variable	
1	minDRll		dEtaFwdJetBJet	
2	dEtaFwdJetClosestLep		Lep3Pt	
3	dEtaFwdJetBJet		maxEtaJet25	
4	dPhiHighestPtSSPair		dEtaFwdJet2BJet	
5	Lep3Pt		dEtaFwdJetClosestLep	
6	maxEtaJet25		minDRll	
7	dEtaFwdJet2BJet		dPhiHighestPtSSPair	
8	nJetEta1		nJet25_Recl	
9	nJet25_Recl		nJetEta1	
10	lepCharge		lepCharge	
1	dEtaFwdJetClosestLep		maxEtaJet25	
2	minDRll		dEtaFwdJet2BJet	
3	maxEtaJet25		dEtaFwdJetBJet	
4	dPhiHighestPtSSPair		Lep2Pt	
5	Lep2Pt		dEtaFwdJetClosestLep	
6	dEtaFwdJetBJet		minDRll	
7	dEtaFwdJet2BJet		nJet25_Recl	
8	nJetEta1		dPhiHighestPtSSPair	
9	nJet25		nJetEta1	
10	lepCharge		lepCharge	

**Table 6.12:** Input variables ranking for BDTG classifiers for the trainings in the  $2lss$  channel (first section) and  $3l$  channel (second section). For both trainings the rankings show almost the same five variables in the first places.

2996        The improvement in the discrimination performance provided by the additional  
 2997        variables is about 1%, so it was decided not to include them in the procedure. Table  
 2998        6.13 shows the ROC-integral for all the testing cases performed.

	ROC-integral	
	$t\bar{t}V$	$t\bar{t}$
base 10 var	0.848	0.777
+ fwdJetPUID	0.849	0.777
+ fwdJetPt25	0.856	0.787
12 var	0.856	0.787

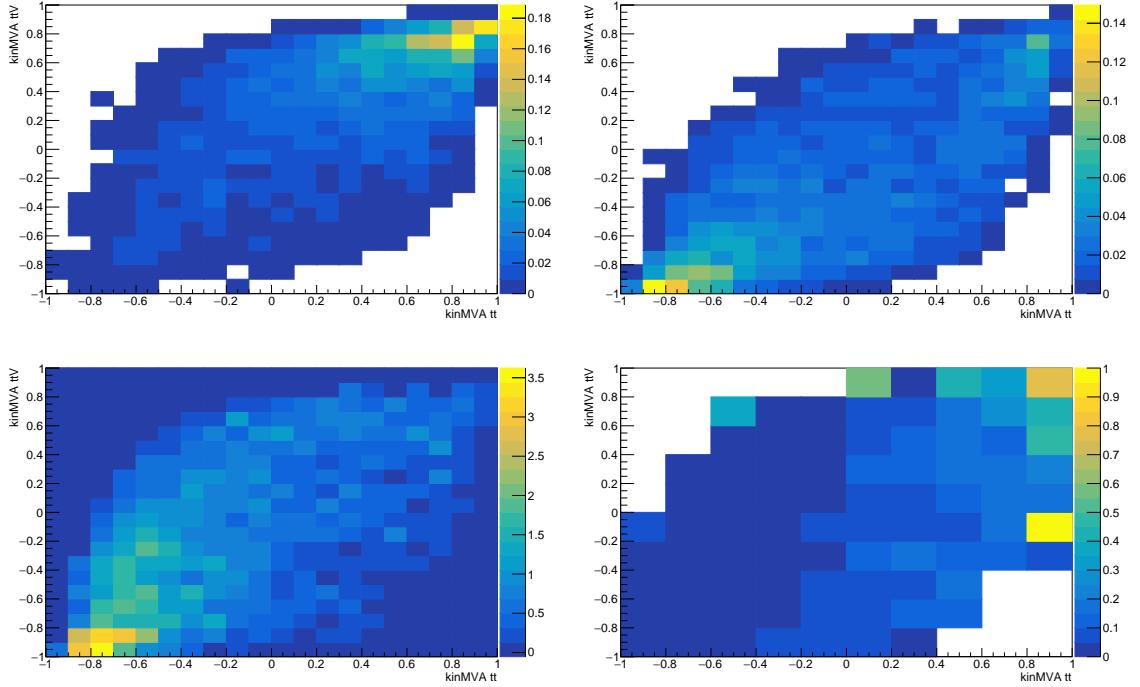
**Table 6.13:** ROC-integral for all the testing cases performed in the evaluation of the additional variables discriminating power. The improvement in the discrimination performance provided by the additional variables is about 1% .



**Figure 6.20:** Additional discriminating variables distributions for  $t\bar{t}V$  training (top row) and  $t\bar{t}$  training (bottom row) in the  $3l$  channel. The origin of the jets in the forward jet identification distribution is tagged as 0 for *pileup jets* while *primary vertex jets* are tagged as 1.

### 2999 6.9.5 Signal extraction procedure

3000 Once the two BDTG classifiers, introduced in the previous section, are trained against  
 3001 the dominant backgrounds in each channel, they are used to classify the events in the  
 3002 samples; their outputs are then used to evaluate the signal cross section limits in a  
 3003 fit to the classifier shape. Figure 6.21 shows the expected output distributions in a  
 3004 2D plane of one training vs. the other, i.e.,  $t\bar{t}V$  vs.  $t\bar{t}$ . Top row shows the 2D planes  
 3005 for  $tHq$  and  $tHW$  signals, while the bottom left plot shows the corresponding 2D

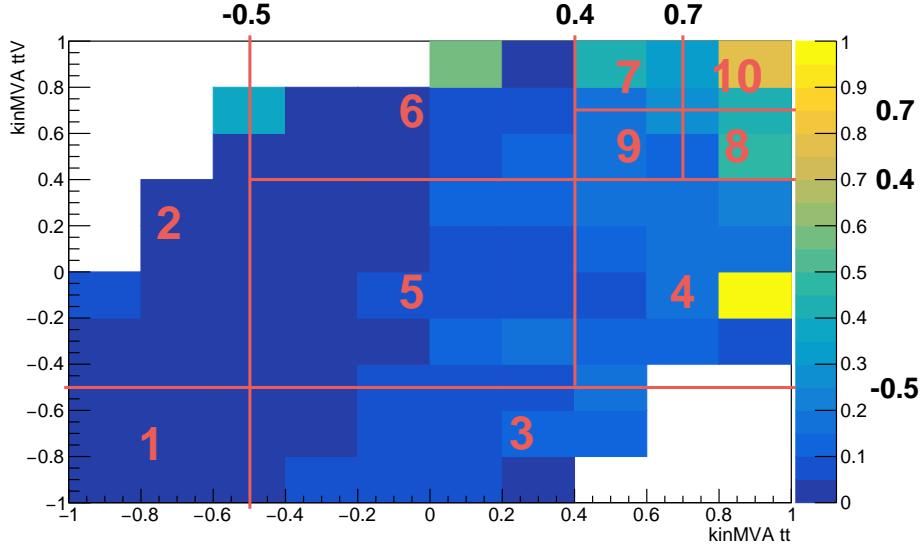


**Figure 6.21:** BDT classifier output planes (training vs  $t\bar{t}$  on x-axis and vs  $t\bar{t}V$  on y-axis) for the  $tHq$  and  $tHW$  signals (top row), and for the combined backgrounds (bottom left). Bottom right: S/B ratio (combining  $tHq$  and  $tHW$ ) in the same plane. Plots are for  $3l$  channel.

3006 plane for the combined backgrounds, which are evaluated as in the final background  
 3007 prediction, i.e., these are not the samples used in the BDTG training and this includes  
 3008 data-driven backgrounds. The signal (combining of  $tHq$  and  $tHW$ ) to background  
 3009 ratio (S/B) is showed in the bottom right plot of Figure 6.21.

3010 Each event is now classified into one of ten 2D-bins according to its position in the  
 3011 plane, as shown in Figure 6.22. The number of bins is chosen such that no bins are  
 3012 entirely empty for any process. The bin boundary positions and number of bins have  
 3013 been studied and optimized with respect to the expected limit on the signal strength  
 3014 (see Sec. 6.9.6).

3015 From this event categorization, a 1D histogram of expected distribution is pro-  
 3016 duced for each signal and background process, and fit to the observed data (or the



**Figure 6.22:** Binning overlaid on the S/B ratio map on the plane of classifier outputs.

3017 Asimov dataset for expected limits).

### 3018 6.9.6 Binning and selection optimization

3019 The effect of the choice of pre-selection cuts and the number of bins of the 1D his-  
 3020 togram on the cross section limit is evaluated by varying the most important cuts and  
 3021 re-calculating the limit in each case. In this analysis, the optimization was performed  
 3022 in the  $3l$  channel, by evaluating the upper limits on the  $tHq + tHW$  expected signal  
 3023 strength only (without  $t\bar{t}H$  component), always evaluated at  $\kappa_t = -1.0$ ,  $\kappa_V = 1.0$ .

3024 Table 6.14 shows several explored variations, compared with a baseline; the base-  
 3025 line is similar to the selection reported in Table 6.6 but only a loose CSV jet and a Z  
 3026 veto of  $\pm 10$  GeV are required.

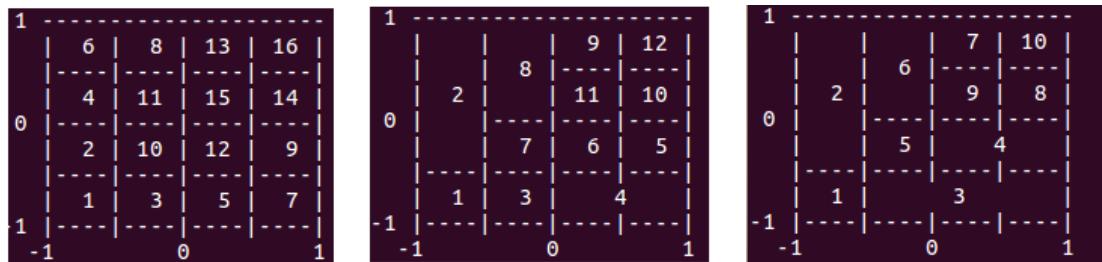
3027 The optimal limit is found when requiring a slightly tighter selection with respect  
 3028 to the baseline. The optimal selection is reported in Table 6.6.

3029 The signal strength limit also depends on the chosen binning in the 2D plane as  
 3030 the S/B ratio varies across the plane, hence, several sizes and binning combinations

Selection	Variation	Expected limit
Baseline		< 2.93
Loose CSV tags	$\geq 1 \rightarrow \geq 2$	< 3.81
Medium CSV tags	$\geq 0 \rightarrow \geq 1$	< 2.76
Light forward jet $\eta$	$\geq 0 \rightarrow \geq 1$	< 2.94
Light forward jet $\eta$	$\geq 0 \rightarrow \geq 1.5$	< 3.00
MET > 30 GeV		< 2.91
Z veto ( $ m_{\ell\ell} - m_Z $ )	$> 10 \text{ GeV} \rightarrow > 15 \text{ GeV}$	< 2.79
One medium CSV + 15 GeV Z veto	combined	< 2.62

**Table 6.14:** Signal strength limit variation as a function of tighter cuts. The baseline selection corresponds to a looser selection compared to the one reported in Table 6.6 where only a CSV-loose  $b$ -jet is required, and the Z veto is loosened to  $\pm 10$  GeV. The optimal selection determined here corresponds to the baseline plus the two variations in the last row.

were tested in order to improve the limit. Figure 6.23 shows some of the binning combinations tested; in the default combination all the bins have the same size, while the best limit was found for a set of 10 bins. The bin borders and the resulting limits are shown in Table 6.15.



**Figure 6.23:** Binning combination scheme.

Combining the optimization of binning and using the tighter pre-selection cuts, the expected limit in the  $3l$  channel alone reaches  $\mathbf{r} < 2.59$ .

A similar binning optimization was made for  $2lss$  channel, including other binning combinations. First, the  $3l$  channel binning was used to estimate the expected limit, then, bin borders were varied to obtain the best possible expected limit. The bin

Number of bins	Bin borders						Expected limit
	$x_1$	$x_2$	$x_3$	$y_1$	$y_2$	$y_3$	
16 (default)	-0.5	0.0	0.5	-0.5	0.0	0.5	< 2.91
16	-0.5	0.3	0.7	-0.5	0.3	0.7	< 2.83
10	-0.5	0.0	0.5	-0.5	0.0	0.5	< 2.93
10	-0.5	0.0	0.7	-0.5	0.0	0.7	< 2.86
10	-0.5	0.0	0.7	-0.5	0.0	0.5	< 2.84
10	-0.5	0.0	0.5	-0.5	0.0	0.7	< 2.87
<b>10</b>	<b>-0.5</b>	<b>0.4</b>	<b>0.7</b>	<b>-0.5</b>	<b>0.4</b>	<b>0.7</b>	<b>&lt; 2.81</b>

**Table 6.15:** Limit variation as a function of bin size. The final bin borders used in the  $3l$  channel are indicated in bold.

3040 borders and the resulting signal strength limits for the same-sign dimuon channel are  
 3041 shown in Table 6.16.

Number of bins	Bin borders						Expected limit
	$x_1$	$x_2$	$x_3$	$y_1$	$y_2$	$y_3$	
16	-0.5	0.4	0.7	-0.5	0.4	0.7	< 1.72
12	-0.5	0.4	0.7	-0.5	0.4	0.7	< 1.72
12	-0.3	0.4	0.7	-0.5	0.4	0.7	< 1.71
12	-0.3	0.3	0.7	-0.5	0.4	0.7	< 1.71
12	-0.3	0.3	0.7	-0.4	0.4	0.7	< 1.70
12	-0.3	0.3	0.7	-0.3	0.4	0.7	< 1.70
12	-0.3	0.3	0.7	-0.3	0.2	0.7	< 1.68
12	-0.3	0.3	0.7	-0.3	0.1	0.7	< 1.70
12	-0.3	0.3	0.7	-0.3	0.2	0.6	< 1.70
10	-0.5	0.4	0.7	-0.5	0.4	0.7	< 1.75
<b>10</b>	<b>-0.3</b>	<b>0.3</b>	<b>0.7</b>	<b>-0.3</b>	<b>0.2</b>	<b>0.6</b>	<b>&lt; 1.69</b>

**Table 6.16:** Limit variation as a function of bin size in the same-sign dimuon channel. (In bold: the final bin borders used in the  $2lss$  channel.)

3042 The expected limit was found to be **r<1.69** for optimized bin borders in 10 bins  
 3043 and optimized pre-selection cuts.

3044 Two additional binning strategies were tested, however, the obtained limits are  
 3045 degraded; they are documented in Appendix C.

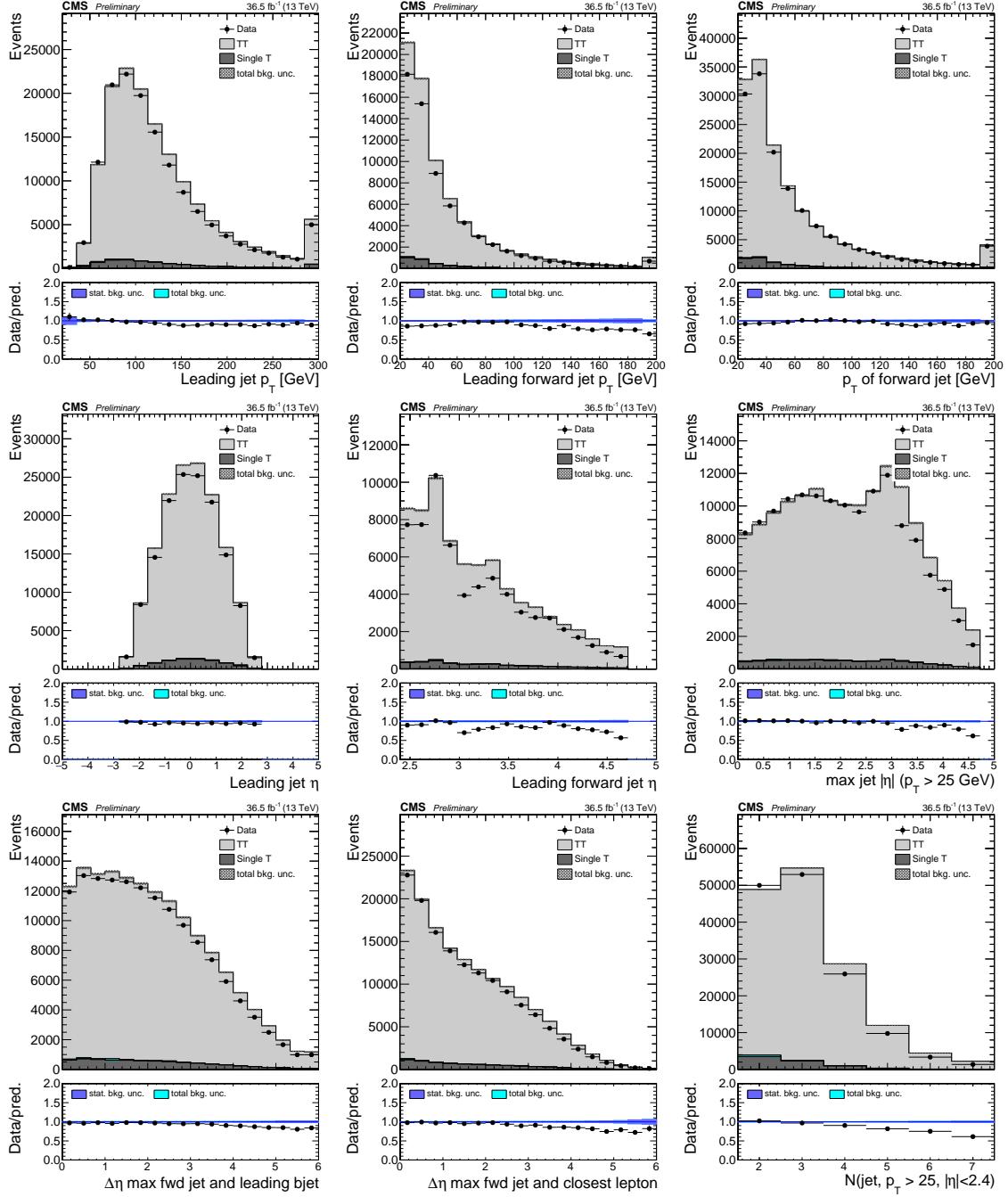
## 3046 6.10 Forward jet mismodeling

3047 As said in previous section, among the features of the  $tHq$  signature that serves as a  
 3048 powerful discriminating variable is the presence of a forward jet; unfortunately, its  $\eta$   
 3049 distribution is poorly modeled in simulation. To estimate the effect of a mismodeled  
 3050 forward jet distribution, a reweighting of the events in simulation based on the nor-  
 3051 malized data/MC ratio in a control region is performed; as a result, an alternative  
 3052 shape of the BDT output distributions that reflects a hypothetical perfect data/MC  
 3053 agreement is derived.

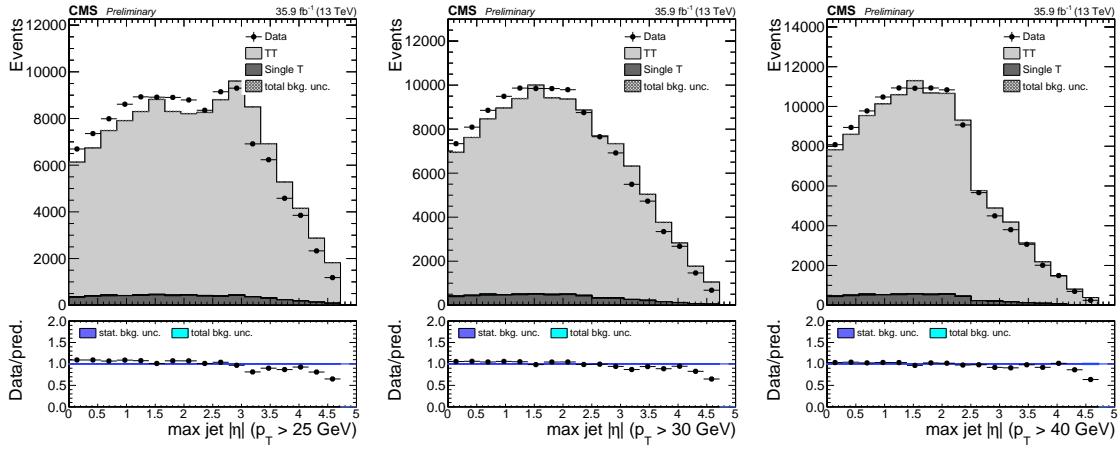
3054 Using a sample of dileptonic  $t\bar{t}$  events, the control region is defined by requiring  
 3055 two opposite-sign tight leptons in the  $e\mu$  channel, with at least two jets and at least  
 3056 one medium CSV tagged jet. (Otherwise the selection is identical to the same-sign  
 3057  $e^\pm\mu^\pm$  channel selection). Some distributions related to the forward jet for MC and  
 3058 data are shown in Figure 6.24.

3059 The disagreement of the  $\eta$  distribution of forward jets for a  $p_T$  cut of 25 GeV is  
 3060 well visible especially at higher values of  $|\eta|$ . The multiplicity for central jets is poorly  
 3061 described by the MadgraphMLM sample used here; consistent with other observations  
 3062 of the same sample. The  $t\bar{t}$  background in this analysis is modeled with a data-driven  
 3063 method and these disagreements do not directly affect the  $t\bar{t}$  contribution in the  
 3064 analysis. They do however reflect the expected agreement in these distributions for  
 3065 the irreducible backgrounds and the signal.

3066 The effect of higher  $p_T$  cuts on the forward jet has been studied for three values:  
 3067 25, 30 and 40 GeV. In order to take into account the data/MC disagreement in the  
 3068 high  $\eta$  regions, the events are weighted accordingly to the data/MC ratio of the  
 3069 unity normalized control plots shown in Figure 6.25. The data/MC agreement in the  
 3070 forward jet  $\eta$  distribution improves significantly at higher jet  $p_T$ s.



**Figure 6.24:** Kinematic distributions in the  $t\bar{t}$ -enriched opposite-sign  $e\mu$  selection. Top row, left to right: leading central ( $\eta < 2.4$ ) jet  $p_T$ , leading forward ( $\eta > 2.4$ ) jet  $p_T$ ,  $p_T$  of non-CSV-loose jet with highest  $\eta$  ("light forward jet"). Middle row:  $\eta$  distribution of those same jets. Bottom row:  $\Delta\eta$  between light forward jet and leading CSV-loose tagged jet;  $\Delta\eta$  between light forward jet and closest lepton; number of central jets.



**Figure 6.25:** Pseudorapidity distributions of the most forward, non-CSV-loose tagged jet in the tt-enriched opposite-sign  $e\mu$  selection for the three  $p_T$  cut values studied.

3071     Table 6.17 shows the scale factors obtained for the three  $p_T$  values. The expected  
 3072     limit on cross section in the  $3l$  was used to determine the most appropriate forward  
 3073     jet  $p_T$  cut; higher  $p_T$  cut improves from 1.54 at 25 GeV to 1.51 at 30 GeV and 1.50  
 3074     at 40 GeV. The impact of the data/MC disagreement for forward jet  $\eta$  is observed  
 3075     to reduce with higher  $p_T$  cuts. Figures F.1, F.2 and F.3 show this reduction in the  
 3076     impact of the forward jet  $\eta$  nuisance in the fit.

## 3077     6.11 Signal model

3078     It is worth to remind that the main goal of this analysis is to test the compatibility  
 3079     of points in the parameter space of Higgs-to-vector boson and Higgs-to-top quark  
 3080     couplings. This is achieved by using simulated  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  signal events  
 3081     which are weighted to reflect the impact of the couplings on kinematic distributions,  
 3082     and together with different predictions of the respective production cross sections and  
 3083     branching ratios, to produce limits on the cross section for different values of  $\kappa_V$  and  
 3084      $\kappa_t$ . See Section 6.4.3 and Table A.3 for the set of  $\kappa_t$  and  $\kappa_V$  values generated. The  
 3085     slight shape-dependence of the BDTG classifier outputs as a function of the couplings

$\eta$ range	$p_T > 25$ GeV	$p_T > 30$ GeV	$p_T > 40$ GeV
0 – 0.278	1.0925	1.0566	1.0326
0.278 – 0.556	1.0920	1.0617	1.0407
0.556 – 0.833	1.0675	1.0459	1.0244
0.833 – 1.111	1.0888	1.0593	1.0340
1.111 – 1.389	1.0759	1.0508	1.0322
1.389 – 1.667	1.0109	0.9847	0.9661
1.667 – 1.944	1.0727	1.0448	1.0239
1.944 – 2.222	1.0715	1.0457	1.0169
2.222 – 2.500	1.0112	0.9871	0.9746
2.500 – 2.778	1.0387	0.9942	0.9816
2.778 – 3.056	0.9687	0.9427	0.9200
3.056 – 3.333	0.8137	0.8695	0.9092
3.333 – 3.611	0.9010	0.9387	0.9807
3.611 – 3.889	0.8685	0.8887	0.9213
3.889 – 4.167	0.9277	0.9466	1.0135
4.167 – 4.444	0.8111	0.8278	0.8637
4.444 – 4.722	0.6497	0.6485	0.6367
4.722 – 5.000	1.0000	1.0000	1.0000
Exp. limit ( $\ell\ell\ell$ )	$r < 1.54$	$r < 1.51$	$r < 1.50$

**Table 6.17:** Data/MC scale factors for  $\eta$  distribution of most forward, non-tagged jet with three different  $p_T$  cuts, see Figure 6.25.

3086 is showed in Appendix D.

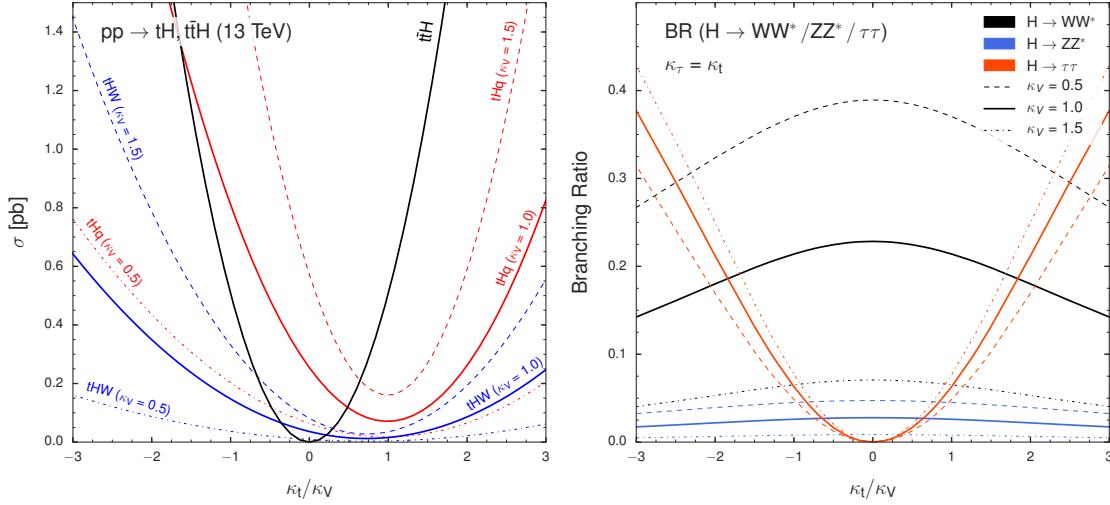
3087 In addition to the  $(\kappa_t, \kappa_V)$  dependence of the  $tHq$  and  $tHW$  production cross  
 3088 sections, due to interferences, the cross section of  $t\bar{t}H$  depends quadratically on  $\kappa_t$   
 3089 according to [158]:

$$\sigma(tHq) = (2.633\kappa_t^2 + 3.578\kappa_V^2 - 5.211\kappa_t\kappa_V) * \sigma_{SM}(tHq), \quad (6.7)$$

$$\sigma(tHW) = (2.909\kappa_t^2 + 2.310\kappa_V^2 - 4.220\kappa_t\kappa_V) * \sigma_{SM}(tHW), \quad (6.8)$$

$$\sigma(t\bar{t}H) = \kappa_t^2 * \sigma_{SM}(t\bar{t}H). \quad (6.9)$$

3090 The Higgs branching fractions to vector bosons depend on  $\kappa_V$ , and the overall



**Figure 6.26:** Scaling of the  $tHq$ ,  $tHW$ , and  $t\bar{H}$  production cross sections (left) and of the  $H \rightarrow WW^*$ ,  $H \rightarrow \tau\tau$ , and  $H \rightarrow ZZ^*$  branching ratios (right), as a function of  $\kappa_t/\kappa_V$ , for three different values of  $\kappa_V$ .

3091 Higgs decay width depend both on  $\kappa_t$  and  $\kappa_V$  when considering resolved top quark  
 3092 loops in the  $H \rightarrow \gamma\gamma$ ,  $H \rightarrow Z\gamma$ , and  $H \rightarrow gg$  decays. The relative contributions from  
 3093  $H \rightarrow WW$ ,  $H \rightarrow ZZ$ , and  $H \rightarrow \tau\tau$  also changes with changing  $\kappa_V$ .

3094 If the Higgs-to-tau coupling modifier ( $\kappa_\tau$ ) is assumed to be equal to  $\kappa_t$ , the relative  
 3095 fractions of  $WW$ ,  $ZZ$ , and  $\tau\tau$  in the event selection will only depend on the ratio of  
 3096  $\kappa_t/\kappa_V$ ; thus, any limit set at any given value of  $\kappa_t/\kappa_V$  is valid for all values of  $\kappa_t$  and  
 3097  $\kappa_V$  with that ratio, and could then be compared with theoretical predictions of cross  
 3098 sections at different values of either modifier. Figure 6.26 shows the  $tHq$ ,  $tHW$  and  
 3099  $t\bar{H}$  cross sections(left) and the Higgs boson branching ratios  $H \rightarrow WW$ ,  $H \rightarrow ZZ$ ,  
 3100 and  $H \rightarrow \tau\tau$  (right) as a function of the  $\kappa_t/\kappa_V$  ratio.

3101 Thus, this analysis sets an upper limit on the combined cross section times branch-  
 3102 ing ratio of  $tHq$ ,  $tHW$ , and  $t\bar{H}$  as a function of the ratio  $\kappa_t/\kappa_V$ .

3103 Similar interpretation can be made if instead of reporting the limits as a function  
 3104 of the  $\kappa_t/\kappa_V$  ratio, they are reported as a function of the relative strength of Higgs-top  
 3105 and Higgs-vector-boson couplings, multiplied by the relative sign

$$f_t = \text{sign}\left(\frac{\kappa_t}{\kappa_V}\right) \times \frac{\kappa_t^2}{\kappa_t^2 + \kappa_V^2}. \quad (6.10)$$

3106 this parameter covers the full space between  $-1.0$  and  $1.0$ , with the SM at  $0.5$ .  
 3107 Absolute values of  $1.0$  or  $0.0$  would correspond to purely Higgs-top and purely Higgs-  
 3108 V couplings, respectively.

3109 Table 6.18 shows the points in the  $\kappa_t/\kappa_V$  and  $f_t$  parameter space that are mapped  
 3110 by the 51 individual  $\kappa_t$  and  $\kappa_V$  points.

3111 The overall Higgs decay width (modified by both  $\kappa_t$  and  $\kappa_V$ ) becomes irrelevant  
 3112 if limits are quoted as absolute cross sections rather than multiples of the expected  
 3113 cross section (which depends on it).

3114 The 1D histograms of events as categorized in regions of the 2D BDTG plane are  
 3115 then used in a maximum likelihood fit of signal and background shapes, where the  
 3116  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  signals are floating with a common signal strength modifier  $r$ ,  
 3117 producing a 95% C.L. upper limit the observed cross section of  $tHq + tHW + t\bar{t}H$ .

3118 This procedure is done separately for each point  $(\kappa_t, \kappa_V)$  where the cross sections  
 3119 and branching fractions are scaled accordingly in each point. Limits at fixed values  
 3120 of  $\kappa_t/\kappa_V$  are by construction identical. Tables G.1–G.3 and G.4–G.6 in Appendix G  
 3121 show the scalings of cross section times branching fraction, as well as branching  
 3122 fractions alone for each of the Higgs decay modes and each of the signal components.

## 3123 6.12 Systematic uncertainties

3124 The uncertainties present in this analysis can be either of statistical nature given  
 3125 the size of the samples and the probabilistic nature of the processes, or of system-  
 3126 atic nature. The systematic uncertainties are associated to theoretical uncertainties  
 3127 originating in the limited knowledge of the processes, and also to experimental uncer-

$f_t$	$\kappa_t/\kappa_V$	$\kappa_V = 0.5$	$\kappa_V = 1.0$	$\kappa_V = 1.5$
-0.973	-6.000	-3.00		
-0.941	-4.000	-2.00		
-0.900	-3.000	-1.50	-3.00	
-0.862	-2.500	-1.25		
-0.800	-2.000	-1.00	-2.00	-3.00
-0.692	-1.500	-0.75	-1.50	
-0.640	-1.333			-2.00
-0.610	-1.250		-1.25	
-0.500	-1.000	-0.50	-1.00	-1.50
-0.410	-0.833			-1.25
-0.360	-0.750		-0.75	
-0.308	-0.667			-1.00
-0.200	-0.500	-0.25	-0.50	-0.75
-0.100	-0.333			-0.50
-0.059	-0.250		-0.25	
-0.027	-0.167			-0.25
0.000	0.000	0.00	0.00	0.00
0.027	0.167			0.25
0.059	0.250		0.25	
0.100	0.333			0.50
0.200	0.500	0.25	0.50	0.75
0.308	0.667			1.00
0.360	0.750		0.75	
0.410	0.833			1.25
0.500	1.000	0.50	1.00	1.50
0.610	1.250		1.25	
0.640	1.333			2.00
0.692	1.500	0.75	1.50	
0.800	2.000	1.00	2.00	3.00
0.862	2.500	1.25		
0.900	3.000	1.50	3.00	
0.941	4.000	2.00		
0.973	6.000	3.00		

**Table 6.18:** The 33 distinct values of  $\kappa_t/\kappa_V$  and  $f_t$  as mapped by the 51  $\kappa_t$  and  $\kappa_V$  points.

3128 tainties originating for instance from the limited resolution of the detectors. In this  
 3129 section, the contributions to the systematic uncertainties from all the sources in this  
 3130 analysis are considered.

3131        Rate uncertainties associated to the application of scaling factors for the affected  
3132    processes, and shape uncertainties which affect not only the normalization but also  
3133    the shape of certain distributions, compose the systematic uncertainties. The latter  
3134    can affect the analysis during the event selection; therefore, these systematic shape  
3135    uncertainties are applied to the simulation samples.

3136        **Experimental uncertainties.**

3137        • *Luminosity.* The measurement of the luminosity delivered by the LHC is af-  
3138    fected by experimental conditions like pileup and the number of protons per  
3139    bunch. Due to variations in the LHC running parameters an uncertainty of  
3140    2.6% is applied.

3141        • *Lepton efficiencies.* Systematic uncertainties in the signal selection efficiency  
3142    arise from correction factors applied to the simulated events in order to better  
3143    match the measured detector performance; also from theoretical uncertainties in  
3144    the modeling of the signal process. Data/MC differences in the trigger efficiency  
3145    accounted with scale factors applied to correct for them, lepton reconstruction  
3146    and identification performance, and lepton selection efficiency carry a combined  
3147    uncertainty of about 5% per lepton.

3148        • *Jets related uncertainties.* Jet energy corrections affect the uncertainty in the  
3149    signal selection efficiency it is evaluated by varying the correction factors within  
3150    their uncertainties and propagating the effects to the final results by recalculat-  
3151    ing the kinematic quantities. The effects of the jet energy scale uncertainties,  
3152     $b$ -tagging efficiency and forward jet mismodeling are evaluated using dedicated  
3153    shape templates derived from a variation of the jet energy scale within its uncer-  
3154    tainty and from varying the  $b$ -tagging forward jet data/MC scale factors within  
3155    their uncertainty.

3156       **Theory uncertainties**

3157       The uncertainties from unknown higher orders of  $tHq$  and  $tHW$  production are  
 3158       estimated from a change in the  $Q^2$  scale of double and half the initial value, evaluated  
 3159       for each point of  $\kappa_t$  and  $\kappa_V$ . The  $t\bar{t}H$  signal component has an uncertainty of about  
 3160        $+5.8/-9.2\%$  from  $Q^2$  scale variations and a further 3.6% from the knowledge of PDFs  
 3161       and  $\alpha_s$  [57]. Uncertainties related to the choice of PDF set and its scale are estimated  
 3162       to be about 3.7% for  $tHq$  and about 4.0% for  $tHW$ .

3163       The theoretical uncertainties from unknown higher orders for  $t\bar{t}W$  and  $t\bar{t}Z$  are  
 3164       12% and 10% respectively; additional uncertainties from the knowledge of PDFs and  
 3165        $\alpha_s$  of about 4% each for  $t\bar{t}W$  and  $t\bar{t}Z$  are estimated.

3166       **Backgrounds**

3167       Besides the theory uncertainties on  $t\bar{t}W$  and  $t\bar{t}Z$ , uncertainties of the smaller  
 3168       irreducible backgrounds and the charge mis-identification estimate are covered with  
 3169       flat normalization uncertainties. The  $WZ$  contribution due to the scale factor is  
 3170       derived during the background estimation using the control region.

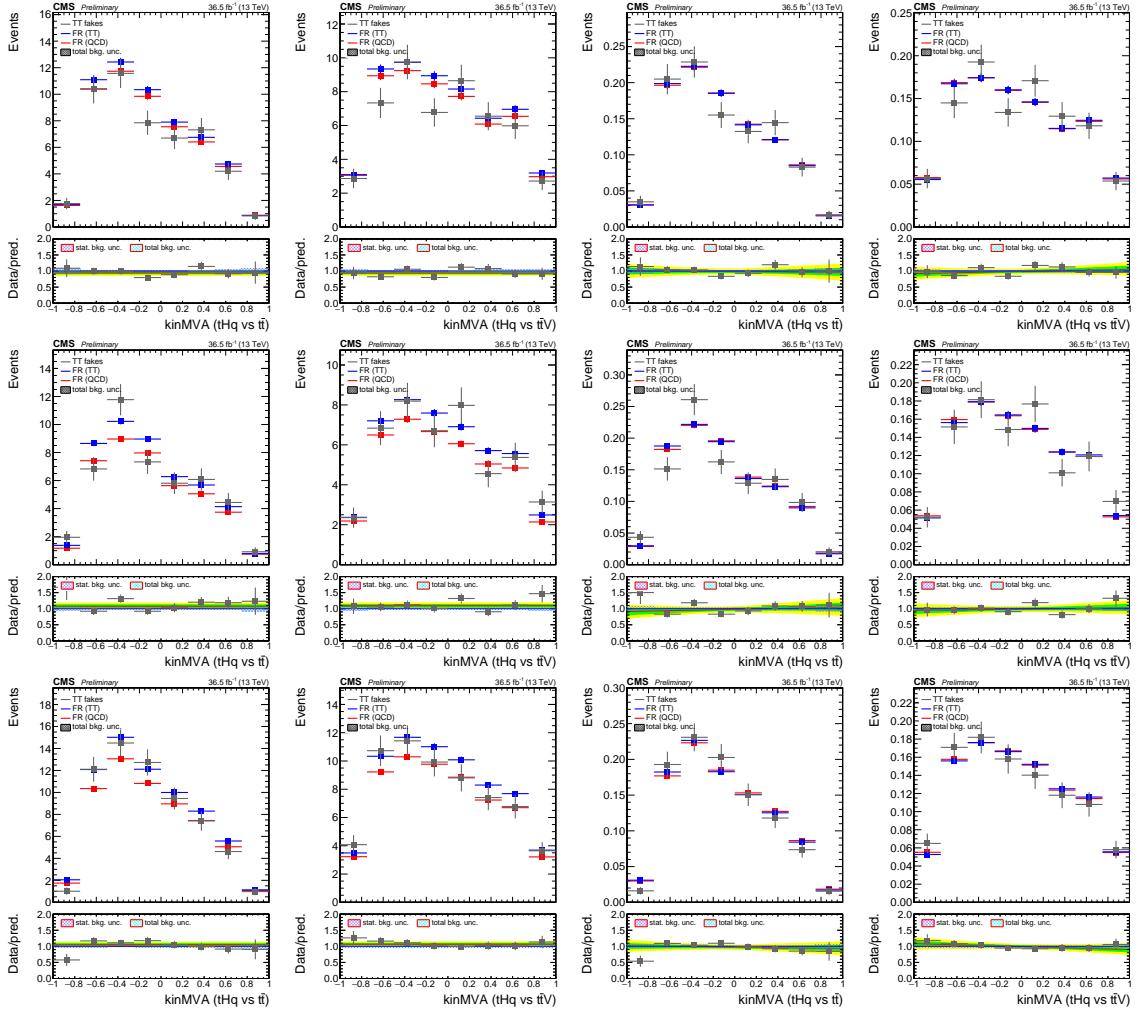
3171       The dominant uncertainty is associated to the estimate of the non-prompt lepton  
 3172       contribution using a fake rate method; the main normalization uncertainty comes from  
 3173       limited statistics in the data control region, and the subtraction of residual prompt  
 3174       lepton contribution as stated in section 6.7.2. Shape variations resembling data/MC  
 3175       differences and deviations in closure test are evaluated as shape uncertainties.

3176       **Fake rate closure uncertainties**

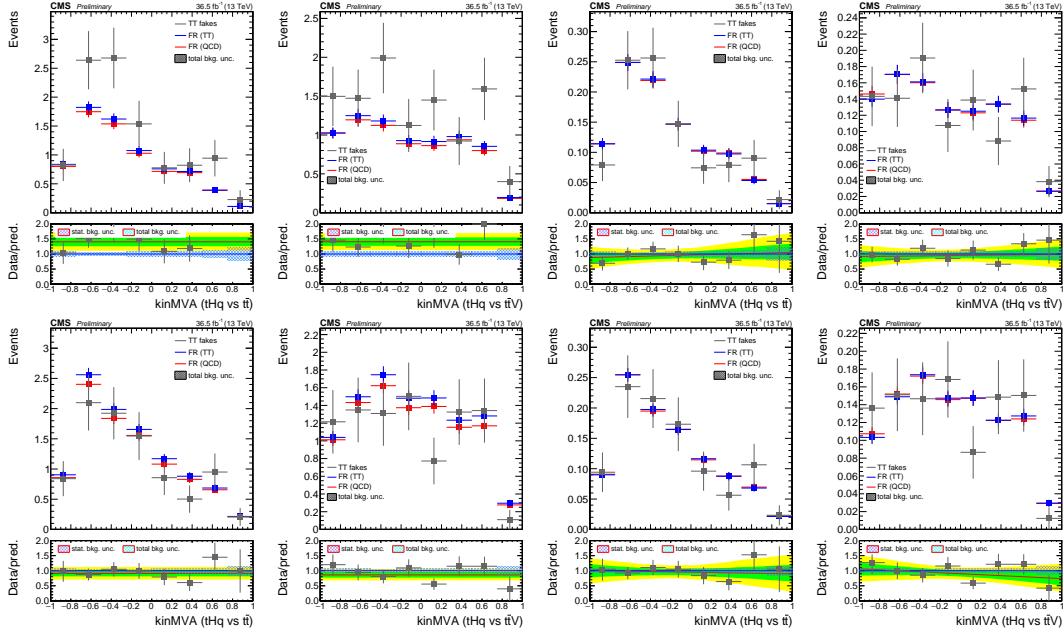
3177       In order to determine the systematic uncertainties associated to the fake rates,  
 3178       the BDTG classifier output shapes from a pure MC estimation of fake leptons (in  
 3179        $t\bar{t}$ ) and from the application of fake-rates as measured in QCD MC, applied in  $t\bar{t}$   
 3180       MC events, are compared. The difference in the resulting normalization and output  
 3181       shapes, for both trainings vs.  $t\bar{t}$  and vs.  $t\bar{t}V$ , are estimated and propagated to the

3182 fit as normalization and shape variations; Figures 6.27 and 6.28 show the results of  
3183 these closure tests.

3184 Table 6.19 list all the systematic uncertainties currently considered in the analysis.



**Figure 6.27:** BDT outputs comparing  $t\bar{t}$  MC to a fake-rate prediction using fake rates measured in QCD MC. Agreement in normalization is estimated from the plots in the two left columns, shape disagreement is estimated from the (normalized) plots in the two right columns. From top to bottom rows: same-sign  $e^\pm \mu^\mp$  selection with electron fakes, same-sign  $e^\pm \mu^\mp$  selection with muon fakes, same-sign  $\mu^\pm \mu^\pm$  selection.



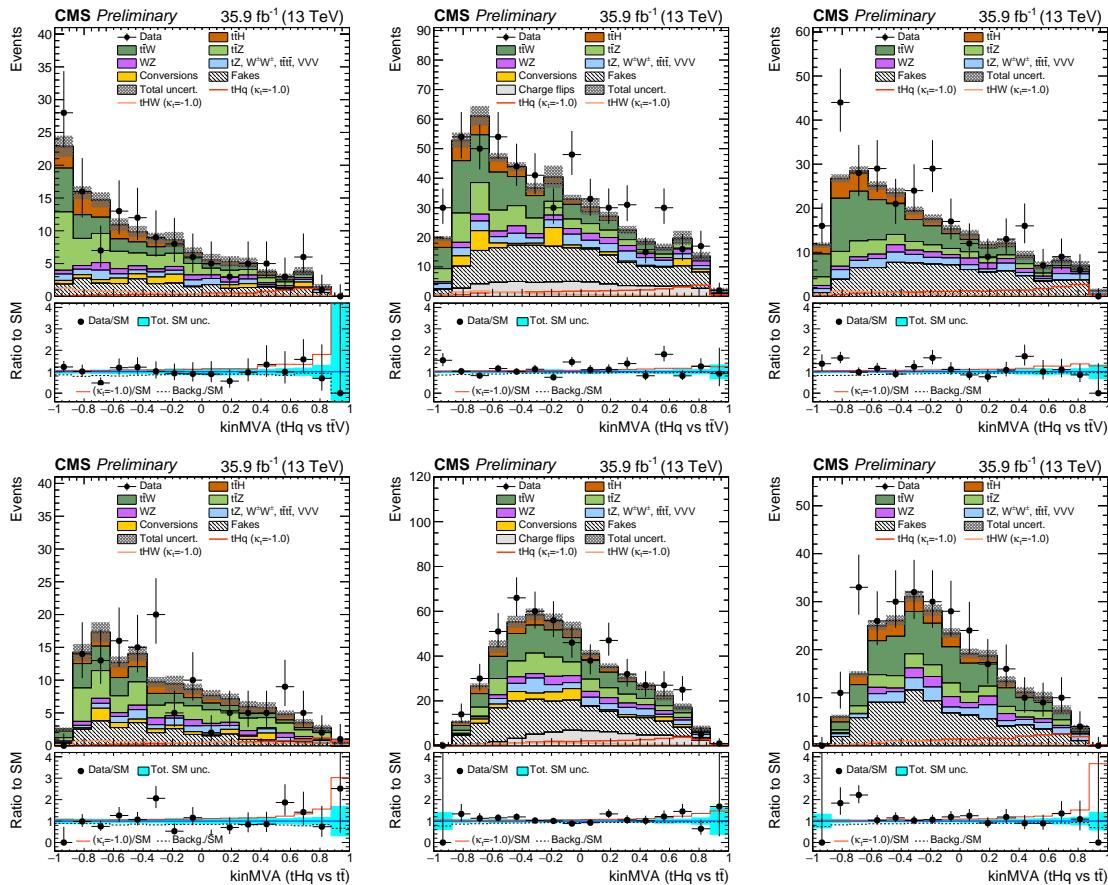
**Figure 6.28:** BDT outputs comparing  $t\bar{t}$  MC to a fake-rate prediction using fake rates measured in QCD MC. Agreement in normalization is estimated from the plots in the two left columns, shape disagreement is estimated from the (normalized) plots in the two right columns. From top to bottom rows: three lepton selection with electron fakes, three lepton selection with muon fakes.

Source	Channel	Size
<b>Experimental uncertainties</b>		
Luminosity	all	1.026
Loose lepton efficiency		1.02 per lepton
Tight lepton efficiency		1.03 per lepton
Trigger efficiency	$\mu^\pm \mu^\pm$ $e^\pm \mu^\pm$ $\ell\ell\ell$	1.01 1.01 1.03
Jet energy scale	all	templates
Forward jet modeling	all	templates, see Table 6.17
_tagging efficiency	all	templates
<b>Theory uncertainties</b>		
$Q^2$ scale ( $tHq$ )	all	0.92–1.06 (depending on $\kappa_t, \kappa_V$ )
$Q^2$ scale ( $tHW$ )	all	0.93–1.05 (depending on $\kappa_t, \kappa_V$ )
$Q^2$ scale ( $t\bar{t}H$ )	all	0.915/1.058
$Q^2$ scale ( $t\bar{t}W$ )	all	1.12
$Q^2$ scale ( $t\bar{t}Z$ )	all	1.11
pdf ( $t\bar{t}H$ )	all	1.036
pdf $gg$ ( $t\bar{t}Z$ )	all	0.966
pdf $q\bar{q}$ ( $t\bar{t}W$ )	all	1.04
pdf $qg$ ( $tHq$ )	all	1.037
pdf $qg$ ( $tHW$ )	all	1.040
<b>Higgs branching fractions</b>		
param_alphaS	all	1.012
param_mB	all	0.981
HiggsDecayWidthTHU_hqq	all	0.988
HiggsDecayWidthTHU_hvv	all	1.004
HiggsDecayWidthTHU_hll	all	1.019
<b>Backgrounds</b>		
$WZ$ control region statistics	$\ell\ell\ell$	1.10
$WZ$ control region backgrounds	$\ell\ell\ell$	1.20
$WZ$ modeling	$\ell\ell\ell$	1.07
$WZ + 2\text{jet}$ background	$\mu^\pm \mu^\pm, e^\pm \mu^\pm$	1.50
Rare SM processes	all	1.50
Charge flips	$e^\pm \mu^\pm$	1.30
<b>Fake rate estimate</b>		
Electron FR measurement		templates
Muon FR measurement		templates
Electron closure	$e^\pm \mu^\pm$	0.94 norm., (0.98 ( $t\bar{t}$ ))/1.07 ( $t\bar{t}V$ )) shape var.
	$\ell\ell\ell$	1.40 norm., (1.09 ( $t\bar{t}$ ))/1.05 ( $t\bar{t}V$ )) shape var.
Muon closure	$\mu^\pm \mu^\pm$	1.07 norm., (0.97 ( $t\bar{t}$ ))/0.91 ( $t\bar{t}V$ )) shape var.
	$e^\pm \mu^\pm$	1.09 norm., (1.06 ( $t\bar{t}$ ))/1.03 ( $t\bar{t}V$ )) shape var.
	$\ell\ell\ell$	1.09 norm., (0.95 ( $t\bar{t}$ ))/0.83 ( $t\bar{t}V$ )) shape var.

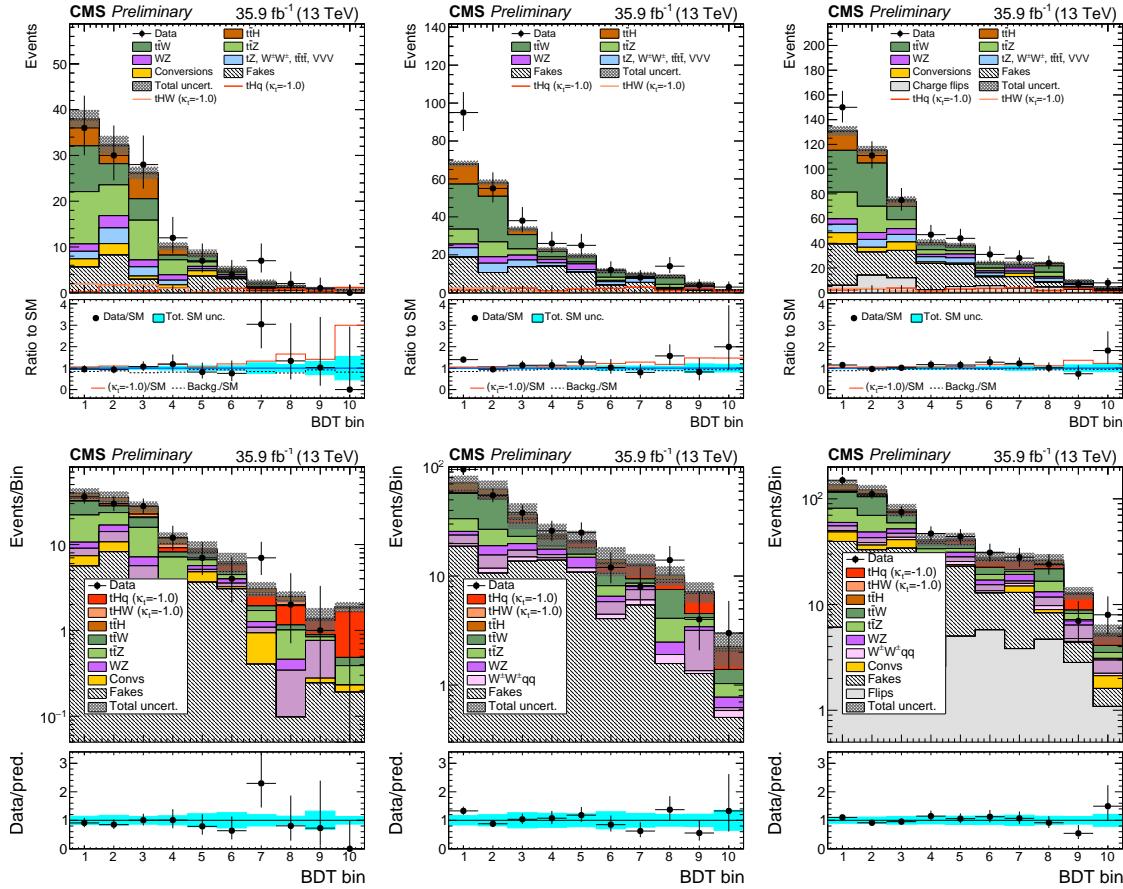
**Table 6.19:** Pre-fit size of systematic uncertainties.

## 3185 6.13 Results

3186 As a result of applying the event pre-selection on the dataset, 127 events are observed  
 3187 in the  $3l$  channel, 280 in the  $2lss \mu^\pm \mu^\pm$  channel and 525 in the  $2lss e^\pm \mu^\pm$  channel  
 3188 as shown in Table 6.8. These events are then classified into one of ten categories,  
 3189 depending on the output of the two BDTG classifiers and according to the optimized  
 binning strategy.



**Figure 6.29:** Pre-fit BDT classifier outputs, for the three-lepton channel (left),  $e^\pm \mu^\pm$  (center), and  $\mu^\pm \mu^\pm$  (right), for  $35.9 \text{ fb}^{-1}$ , for training against  $t\bar{t}V$  (top row) and against  $t\bar{t}$  (bottom row). In the box below each distribution, the ratio of the observed and predicted event yields is shown. The shape of the two  $tH$  signals for  $\kappa_t = -1.0$  is shown, normalized to their respective cross sections for  $\kappa_t = -1.0, \kappa_V = 1.0$ . The grey band represents the unconstrained (pre-fit) statistical and systematical uncertainties.



**Figure 6.30:** Expected (pre-fit) distributions in the final binning used for the signal extraction, for (from left to right) the three lepton channel, the  $\mu^{\pm}\mu^{\pm}$  channel, and the  $e^{\pm}\mu^{\pm}$  channel. Linear scale (top row), and logarithmic scale (bottom row).

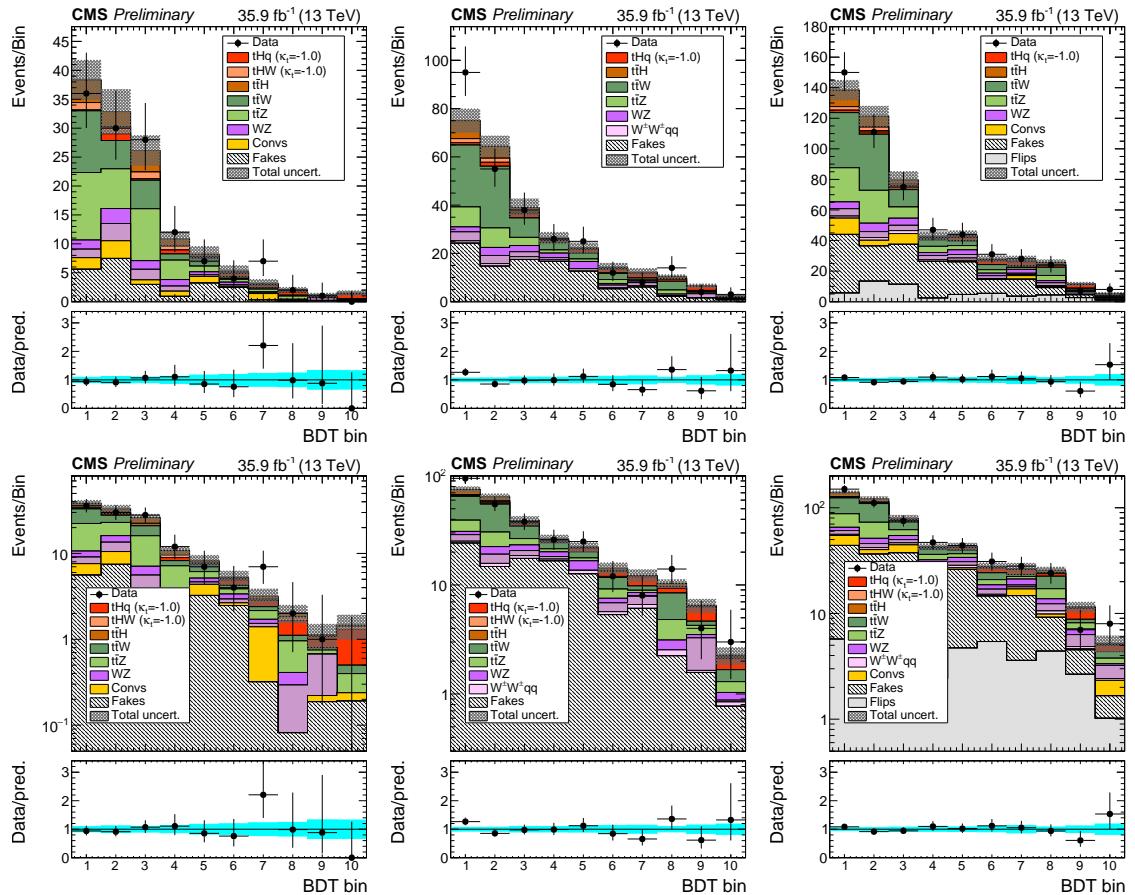
3191     The pre-fit distributions of BDTG outputs are shown in Figure 6.29, while the  
 3192     pre-fit distributions in the final binning used in the signal extraction are shown in  
 3193     Figure 6.30.

3194     The expected signal and background shapes for the distribution in the 1D his-  
 3195     togram (with ten bins) are fit to the observed data in a maximum likelihood fit, for  
 3196     all three channels simultaneously and separately for the signal shapes for each of the  
 3197     33  $\kappa_t/\kappa_V$  coupling configuration points.

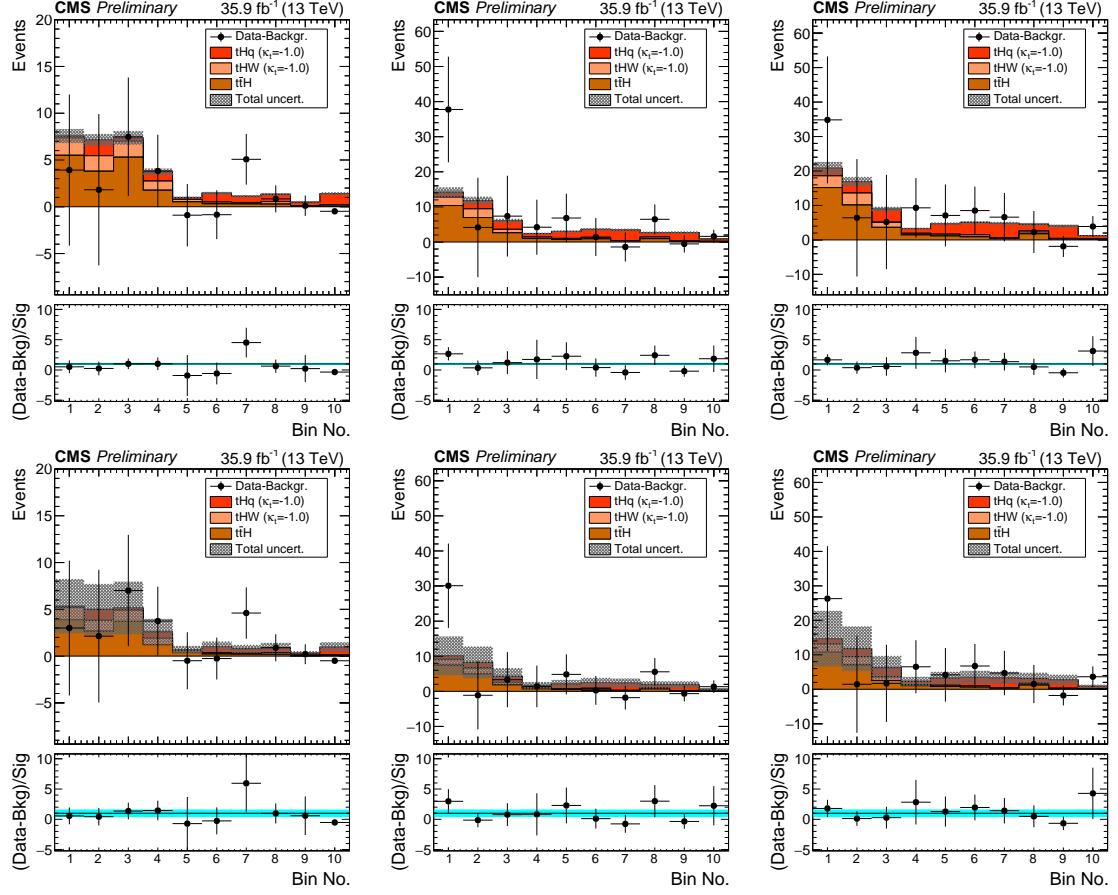
3198     The  $tH$  and  $t\bar{H}$  production cross sections and the Higgs decay branching ratios are  
 3199     modified in each point with the Higgs-top ( $\kappa_t$ ) and Higgs-vector boson ( $\kappa_V$ ) coupling

strength and the Higgs-tau coupling strength modifier ( $\kappa_\tau$ ) is assumed to be equal to  $\kappa_t$ ; the rest of the parameters are assumed to be at the SM predicted values. The combined signal shape is then uniquely defined by the ratio of  $\kappa_t/\kappa_V$ . In the fit, the signal components,  $tH$  and  $t\bar{t}H$ , are floated with a common signal strength modifier (defined as the ratio to the expected cross section) to produce a 95% confidence level (C.L) upper limit on the observed  $tH + t\bar{t}H$  cross section times the combined branching ratio of  $H \rightarrow WW^* + ZZ^* + \tau\tau$ .

The post-fit categorized BDTG output distributions obtained in the maximum likelihood fit to extract the limits, are shown in Figure 6.31.

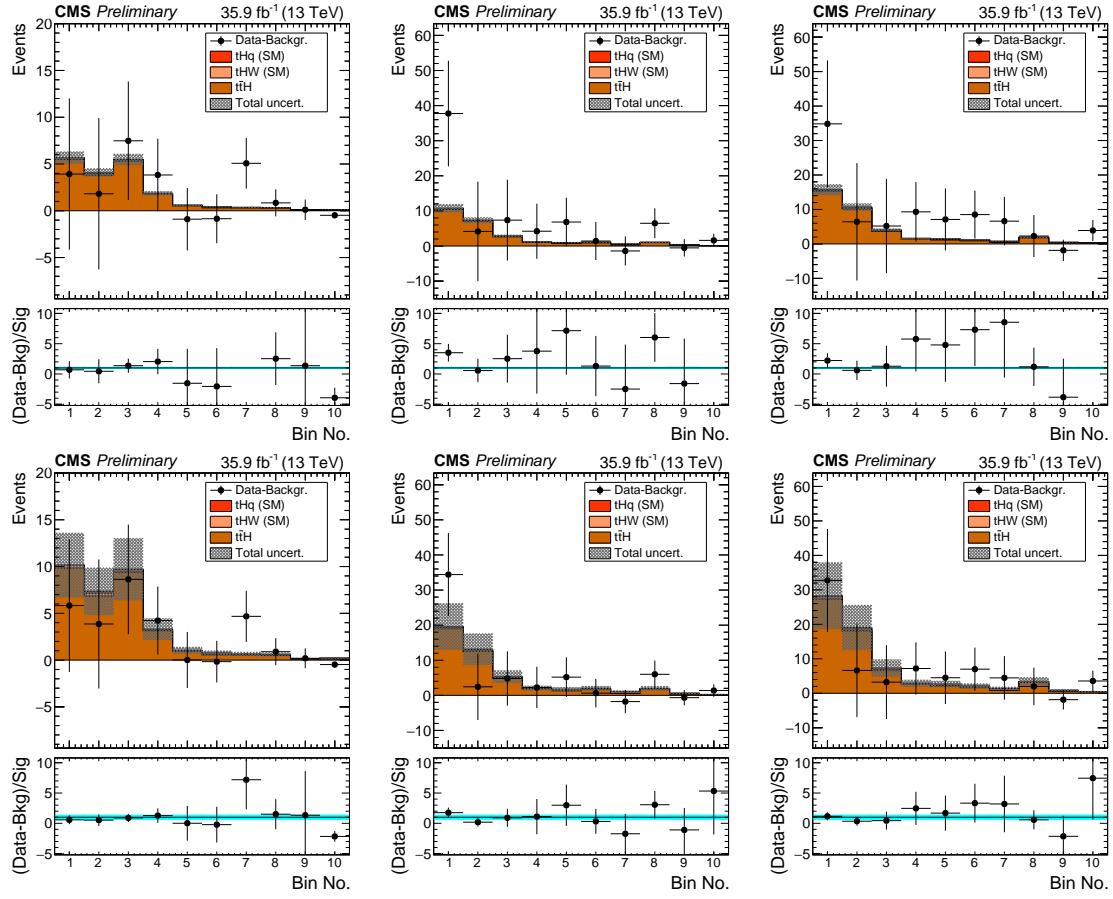


**Figure 6.31:** Post-fit distributions in the final binning used for the signal extraction, for (from left to right) the three lepton channel, the  $\mu^\pm\mu^\pm$  channel, and the  $e^\pm\mu^\pm$  channel. Linear scale (top row), and logarithmic scale (bottom row).



**Figure 6.32:** Background-subtracted pre- (top) and post-fit (bottom) distributions in the final binning used for the signal extraction, for three lepton channel (left), the  $\mu^{\pm}\mu^{\pm}$  channel (center), and the  $e^{\pm}e^{\pm}$  channel (right). For a fit in the inverted couplings scenario ( $\kappa_V = 1, \kappa_t = -1$ ).

3209 As expected, the signal contribution is very small compared to the background  
 3210 ground contribution; however, it is possible to see the signal contribution by subtracting the background from the overall BDT output distributions as shown in Figure  
 3211 6.32 for the inverted coupling scenario ( $\kappa_V = 1, \kappa_t = -1$ ) and Figure 6.33 for the SM-like  
 3212 scenario ( $\kappa_V = 1, \kappa_t = 1$ ).  
 3213



**Figure 6.33:** Background-subtracted pre- (top) and post-fit (bottom) distributions in the final binning used for the signal extraction, for the three lepton channel (left), the  $\mu^\pm\mu^\pm$  channel (center), and the  $e^\pm\mu^\pm$  channel (right). For a fit in the SM-like scenario ( $\kappa_t = \kappa_V = 1$ ).

### 3214 6.13.1 $CL_S$ and cross section limits

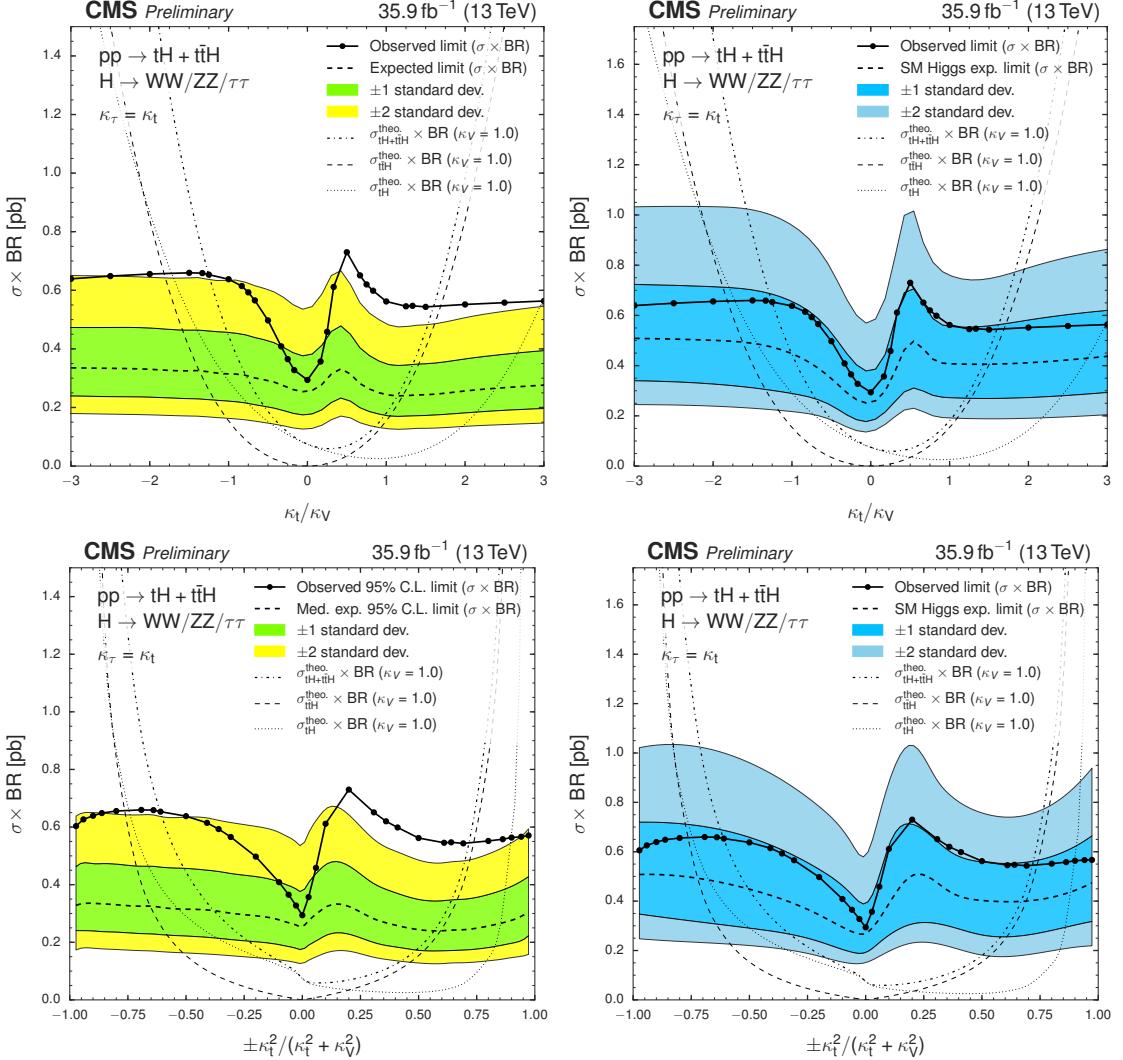
3215 Table 6.20 lists the expected background only, the expected SM-like Higgs signal, and  
 3216 the observed 95% C.L. upper limits on the  $tH + t\bar{t}H$  production cross section times  
 3217  $H \rightarrow WW^* + ZZ^* + \tau\tau$  branching ratio (in pb); the corresponding plots are shown  
 3218 in Figure 6.34 for  $\kappa_V = 1$ . The expected background-only limit is calculated on an  
 3219 Asimov dataset, while the expected SM-like limit is calculated on an Asimov dataset  
 3220 that includes the SM-like  $tH$  and  $t\bar{t}H$  signals.

3221 An excess of more than  $2\sigma$  is observed for the SM configuration ( $\kappa_t/\kappa_V = 1$ ) for the

$f_t$	$\kappa_t/\kappa_V$	Exp. lim.	SM exp.	Obs. lim.	Best fit $\sigma$ [pb]	Best fit $r$
-0.973	-6.000	0.328 $^{+0.136}_{-0.090}$	0.507 $^{+0.206}_{-0.158}$	0.603	0.305 $^{+0.155}_{-0.169}$	0.013 $^{+0.007}_{-0.007}$
-0.941	-4.000	0.335 $^{+0.137}_{-0.098}$	0.509 $^{+0.215}_{-0.166}$	0.627	0.322 $^{+0.157}_{-0.174}$	0.036 $^{+0.018}_{-0.020}$
-0.900	-3.000	0.335 $^{+0.138}_{-0.096}$	0.510 $^{+0.215}_{-0.172}$	0.639	0.334 $^{+0.160}_{-0.173}$	0.075 $^{+0.036}_{-0.039}$
-0.862	-2.500	0.334 $^{+0.139}_{-0.097}$	0.505 $^{+0.217}_{-0.173}$	0.649	0.341 $^{+0.160}_{-0.174}$	0.119 $^{+0.056}_{-0.061}$
-0.800	-2.000	0.330 $^{+0.141}_{-0.095}$	0.500 $^{+0.212}_{-0.176}$	0.656	0.345 $^{+0.165}_{-0.176}$	0.202 $^{+0.097}_{-0.103}$
-0.692	-1.500	0.325 $^{+0.139}_{-0.095}$	0.485 $^{+0.209}_{-0.172}$	0.660	0.340 $^{+0.164}_{-0.176}$	0.369 $^{+0.178}_{-0.191}$
-0.640	-1.333	0.325 $^{+0.139}_{-0.097}$	0.482 $^{+0.210}_{-0.173}$	0.659	0.334 $^{+0.169}_{-0.174}$	0.456 $^{+0.231}_{-0.238}$
-0.610	-1.250	0.321 $^{+0.140}_{-0.095}$	0.474 $^{+0.210}_{-0.169}$	0.653	0.328 $^{+0.164}_{-0.177}$	0.505 $^{+0.252}_{-0.272}$
<b>-0.500</b>	<b>-1.000</b>	<b>0.315 <math>^{+0.142}_{-0.093}</math></b>	<b>0.450 <math>^{+0.213}_{-0.160}</math></b>	<b>0.638</b>	<b>0.304 <math>^{+0.175}_{-0.176}</math></b>	<b>0.685 <math>^{+0.395}_{-0.396}</math></b>
-0.410	-0.833	0.312 $^{+0.138}_{-0.095}$	0.424 $^{+0.210}_{-0.147}$	0.615	0.276 $^{+0.168}_{-0.177}$	0.819 $^{+0.498}_{-0.526}$
-0.360	-0.750	0.307 $^{+0.138}_{-0.093}$	0.409 $^{+0.200}_{-0.136}$	0.593	0.256 $^{+0.170}_{-0.176}$	0.874 $^{+0.581}_{-0.601}$
-0.308	-0.667	0.301 $^{+0.138}_{-0.092}$	0.384 $^{+0.198}_{-0.124}$	0.566	0.231 $^{+0.165}_{-0.174}$	0.915 $^{+0.655}_{-0.689}$
-0.200	-0.500	0.292 $^{+0.136}_{-0.090}$	0.345 $^{+0.181}_{-0.109}$	0.497	0.166 $^{+0.163}_{-0.162}$	0.895 $^{+0.879}_{-0.871}$
-0.100	-0.333	0.278 $^{+0.132}_{-0.086}$	0.303 $^{+0.156}_{-0.092}$	0.409	0.092 $^{+0.157}_{-0.092}$	0.679 $^{+1.159}_{-0.679}$
-0.059	-0.250	0.268 $^{+0.129}_{-0.083}$	0.283 $^{+0.152}_{-0.085}$	0.365	0.059 $^{+0.148}_{-0.059}$	0.515 $^{+1.285}_{-0.515}$
-0.027	-0.167	0.260 $^{+0.125}_{-0.081}$	0.266 $^{+0.135}_{-0.077}$	0.328	0.029 $^{+0.142}_{-0.029}$	0.297 $^{+1.434}_{-0.297}$
0.000	0.000	0.254 $^{+0.123}_{-0.079}$	0.252 $^{+0.123}_{-0.073}$	0.294	0.000 $^{+0.132}_{-0.000}$	0.002 $^{+1.776}_{-0.002}$
0.027	0.167	0.275 $^{+0.132}_{-0.086}$	0.284 $^{+0.148}_{-0.084}$	0.357	0.040 $^{+0.154}_{-0.040}$	0.650 $^{+2.514}_{-0.650}$
0.059	0.250	0.297 $^{+0.141}_{-0.093}$	0.329 $^{+0.171}_{-0.099}$	0.458	0.119 $^{+0.183}_{-0.119}$	2.015 $^{+3.098}_{-2.015}$
0.100	0.333	0.322 $^{+0.148}_{-0.099}$	0.405 $^{+0.220}_{-0.135}$	0.611	0.246 $^{+0.166}_{-0.184}$	4.147 $^{+2.802}_{-3.103}$
0.200	0.500	0.324 $^{+0.141}_{-0.096}$	0.505 $^{+0.212}_{-0.181}$	0.730	0.413 $^{+0.150}_{-0.177}$	5.982 $^{+2.174}_{-2.559}$
0.308	0.667	0.281 $^{+0.122}_{-0.082}$	0.462 $^{+0.172}_{-0.159}$	0.651	0.382 $^{+0.136}_{-0.144}$	4.186 $^{+1.492}_{-1.574}$
0.360	0.750	0.268 $^{+0.116}_{-0.079}$	0.442 $^{+0.160}_{-0.154}$	0.620	0.364 $^{+0.130}_{-0.135}$	3.392 $^{+1.214}_{-1.253}$
0.410	0.833	0.258 $^{+0.112}_{-0.075}$	0.427 $^{+0.162}_{-0.147}$	0.599	0.351 $^{+0.127}_{-0.130}$	2.754 $^{+0.999}_{-1.022}$
<b>0.500</b>	<b>1.000</b>	<b>0.244 <math>^{+0.105}_{-0.072}</math></b>	<b>0.401 <math>^{+0.154}_{-0.137}</math></b>	<b>0.562</b>	<b>0.328 <math>^{+0.118}_{-0.121}</math></b>	<b>1.821 <math>^{+0.657}_{-0.671}</math></b>
0.610	1.250	0.240 $^{+0.104}_{-0.070}$	0.394 $^{+0.154}_{-0.133}$	0.545	0.315 $^{+0.118}_{-0.119}$	1.072 $^{+0.399}_{-0.403}$
0.640	1.333	0.242 $^{+0.105}_{-0.071}$	0.398 $^{+0.156}_{-0.136}$	0.547	0.316 $^{+0.122}_{-0.121}$	0.921 $^{+0.354}_{-0.352}$
0.692	1.500	0.244 $^{+0.106}_{-0.071}$	0.401 $^{+0.159}_{-0.136}$	0.543	0.312 $^{+0.120}_{-0.120}$	0.678 $^{+0.262}_{-0.261}$
0.800	2.000	0.256 $^{+0.109}_{-0.075}$	0.416 $^{+0.169}_{-0.138}$	0.552	0.311 $^{+0.121}_{-0.127}$	0.317 $^{+0.123}_{-0.129}$
0.862	2.500	0.268 $^{+0.114}_{-0.078}$	0.433 $^{+0.169}_{-0.142}$	0.558	0.310 $^{+0.127}_{-0.130}$	0.170 $^{+0.070}_{-0.072}$
0.900	3.000	0.276 $^{+0.118}_{-0.080}$	0.442 $^{+0.177}_{-0.144}$	0.563	0.308 $^{+0.128}_{-0.134}$	0.102 $^{+0.042}_{-0.044}$
0.941	4.000	0.290 $^{+0.122}_{-0.084}$	0.459 $^{+0.184}_{-0.149}$	0.566	0.304 $^{+0.134}_{-0.140}$	0.046 $^{+0.020}_{-0.021}$
0.973	6.000	0.306 $^{+0.122}_{-0.081}$	0.474 $^{+0.192}_{-0.150}$	0.571	0.300 $^{+0.131}_{-0.150}$	0.016 $^{+0.007}_{-0.008}$

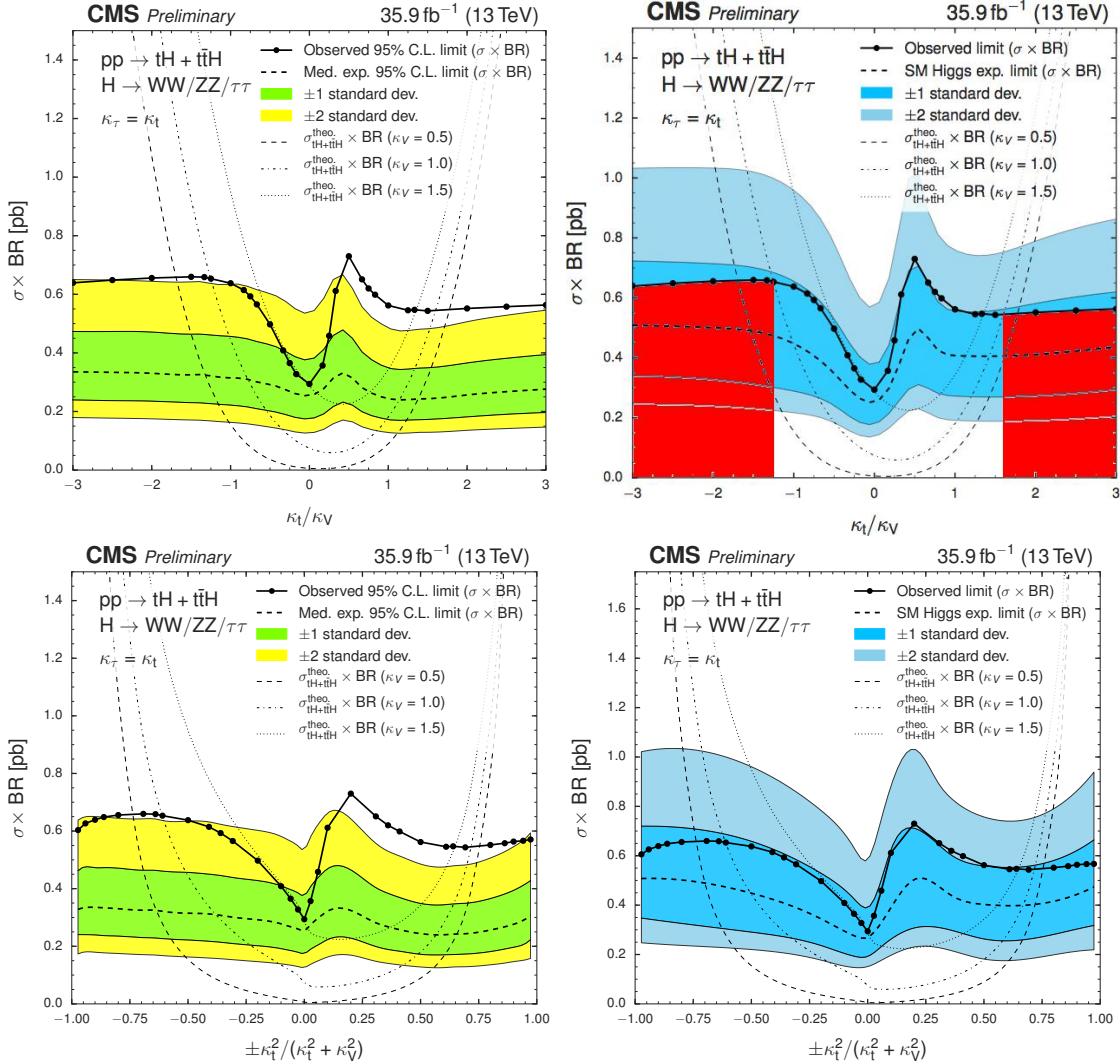
**Table 6.20:** Expected (for background only, and for a SM-like Higgs signal) and observed 95% C.L. upper limits (in pb), and best fit signal strength  $r$  and corresponding best fit cross section for the combined  $tH + t\bar{t}H$  cross section times modified branching ratio for the combination of all three channels, for different values of  $\kappa_t/\kappa_V$  or the equivalent  $f_t$  numbers.

background-only expected limit; however, the inclusion of the SM-like  $tH$  and  $t\bar{t}H$  signals reveals that the excess is actually about  $1\sigma$ ; furthermore, looking at  $\kappa_t/\kappa_V = 0$ , i.e., the  $t\bar{t}H$  component in the signal is zero, it is evident that the origin of the excess is mostly due to the presence of the  $t\bar{t}H$  component in the signal, given that the



**Figure 6.34:** Left (Right): Expected background-only (SM-like including  $t\bar{t}H$  and  $tH$  signals) and observed asymptotic limits on the combined  $tH + t\bar{t}H$  cross section times modified BR as a function of  $\kappa_t/\kappa_V$  (top) and  $\text{sign}(\kappa_t/\kappa_V) \times \frac{\kappa_t^2}{(\kappa_t^2 + \kappa_V^2)}$  (bottom) for the combination of three lepton channel,  $\mu^\pm\mu^\pm$ , and  $e^\pm\mu^\pm$  channel.

3226 deviation of the observed limit from the expected one is much smaller than  $1\sigma$ ; this is  
 3227 consistent with the results presented in Reference [149]. It is also evident that, given  
 3228 the dependence of the  $t\bar{t}H$  cross section on  $\kappa_t^2$ , the source of the asymmetry in both,  
 3229 background-only and SM-like, limits is induced by the  $tH$  component of the signal.  
 3230 Comparing the observed upper limit with the theoretical prediction of the  $tH +$



**Figure 6.35:** Left (Right): Expected background-only (SM-like including  $t\bar{t}H$  and  $tH$  signals) and observed asymptotic limits on the combined  $tH + t\bar{t}H$  cross section times modified BR as a function of  $\kappa_t/\kappa_V$  (top) and  $\text{sign}(\kappa_t/\kappa_V) \times \frac{\kappa_t^2}{(\kappa_t^2 + \kappa_V^2)}$  (bottom) for the combination of three lepton channel,  $\mu^\pm\mu^\pm$ , and  $e^\pm\mu^\pm$  channel. Theoretical  $tH + t\bar{t}H$  cross section curves have been included for  $\kappa_V = 0.5, 1.0, 1.5$ . Red areas on the top right plot correspond to the excluded regions.

3231     $t\bar{t}H$  cross section times BR for  $\kappa_V = 1.0$  constrains the allowed range of coupling  
 3232    configurations  $\kappa_t/\kappa_V$  to between about -1.25 and +1.60. as shown in the top right  
 3233    plot in Figure 6.35.

3234    The observed limit of about 0.64 pb on a signal shape expected for  $\kappa_t/\kappa_V = -1.0$

Scenario	Channel	Obs. Limit (pb)	Exp. Limit (pb)		
			Median	$\pm 1\sigma$	$\pm 2\sigma$
$\kappa_t/\kappa_V = -1$	$\mu^\pm\mu^\pm$	1.00	0.58	[0.42, 0.83]	[0.31, 1.15]
	$e^\pm\mu^\pm$	0.84	0.54	[0.39, 0.76]	[0.29, 1.03]
	$\ell\ell\ell$	0.70	0.38	[0.26, 0.56]	[0.19, 0.79]
	Combined	<b>0.64</b>	<b>0.32</b>	[0.22, 0.46]	[0.16, 0.64]
$\kappa_t/\kappa_V = 1$ (SM-like)	$\mu^\pm\mu^\pm$	0.87	0.41	[0.29, 0.58]	[0.22, 0.82]
	$e^\pm\mu^\pm$	0.59	0.37	[0.26, 0.53]	[0.20, 0.73]
	$\ell\ell\ell$	0.54	0.31	[0.22, 0.43]	[0.16, 0.62]
	Combined	<b>0.56</b>	<b>0.24</b>	[0.17, 0.35]	[0.13, 0.49]

**Table 6.21:** Expected and observed 95% C.L. upper limits on the  $tH + t\bar{t}H$  production cross section times  $H \rightarrow WW^* + \tau\tau + ZZ^*$  branching ratio for a scenario of inverted couplings ( $\kappa_t/\kappa_V = -1.0$ , top rows) and for a standard-model-like signal ( $\kappa_t/\kappa_V = 1.0$ , bottom rows), in pb. The expected limit is calculated on a background-only Asimov dataset and quoted with  $\pm 1\sigma$  and  $\pm 2\sigma$  probability ranges.

Scenario	Channel	Obs. Limit	Exp. Limit				
			$-2\sigma$	$-1\sigma$	Median	$+1\sigma$	$+2\sigma$
$\kappa_V = 1.0$	$\mu^\pm\mu^\pm$	2.3	0.71	0.94	1.32	1.88	2.60
	$e^\pm\mu^\pm$	1.9	0.65	0.87	1.21	1.71	2.32
	$\ell\ell\ell$	1.6	0.43	0.59	0.86	1.26	1.78
	Combined ( $\mu\mu, 3\ell$ )	<b>1.6</b>	0.40	0.54	<b>0.78</b>	1.12	1.57
	Combined ( $\mu\mu, e\mu, 3\ell$ )	<b>1.4</b>	0.37	0.50	<b>0.71</b>	1.03	1.43
(SM)	$\mu^\pm\mu^\pm$	4.9	1.20	1.61	2.27	3.24	4.54
	$e^\pm\mu^\pm$	3.3	1.10	1.48	2.07	2.95	4.06
	$\ell\ell\ell$	3.0	0.91	1.22	1.73	2.49	3.47
	Combined ( $\mu\mu, 3\ell$ )	<b>3.4</b>	0.79	1.07	<b>1.51</b>	2.17	3.01
	Combined ( $\mu\mu, e\mu, 3\ell$ )	<b>3.1</b>	0.71	0.96	<b>1.36</b>	1.94	2.70

**Table 6.22:** Expected and observed CL<sub>S</sub> limits (at 95% C.L.) on the signal strength of combined  $tH + t\bar{t}H$  production in each channel, and for different combinations of them, for a scenario with inverted couplings ( $\kappa_V = 1.0$ ,  $\kappa_t = -1.0$ , top section), and for the standard model ( $\kappa_V = \kappa_t = 1.0$ , bottom section). Numbers are for  $35.9 fb^{-1}$ .

and for the combination of all three channels, corresponds to 1.4 times the expected  $tH + t\bar{t}H$  cross section with  $\kappa_t = -1.0$ ,  $\kappa_V = 1.0$ . In the SM scenario ( $\kappa_t/\kappa_V = 1.0$ ), the observed upper limit on the cross section times branching ratio is 0.56 pb, corresponding to 3.1 times the expected SM cross section of  $tH + t\bar{t}H$ . The summary of the results for the ITC and SM-like scenarios split by channel are presented in Table

3240 6.21, whereas, the summary of the expected and observed CL<sub>S</sub> limits (at 95% C.L.)  
 3241 on the signal strength of combined  $tH + t\bar{t}H$  production in each channel, and for  
 3242 different combinations thereof, for the ITC and SM-like scenarios are presented in  
 3243 Table 6.26.

3244 **6.13.2 Best fit**

3245 The best-fit results for the signal strength in all the 33  $\kappa_t/\kappa_V$  configurations are also  
 3246 listed in Table 6.20; the inverted top coupling (ITC) and the SM-like scenarios are  
 3247 highlighted there and summarized in Table 6.23. The individual contributions from  
 3248 all the channels to the best-fit signal strength for the SM-like Higgs signal are listed  
 3249 in Table 6.24.

Scenario	Best fit signal strength	Best fit $\sigma \times BR$	Significance Obs.(exp.)
$\kappa_t/\kappa_V = -1.0$	$0.68 \pm 0.40$	$0.30 \pm 0.18$ pb	$1.70\sigma(2.51\sigma)$
$\kappa_t/\kappa_V = 1.0$	$1.82^{+0.66}_{-0.67}$	$0.33 \pm 0.12$ pb	$2.73\sigma(1.50\sigma)$

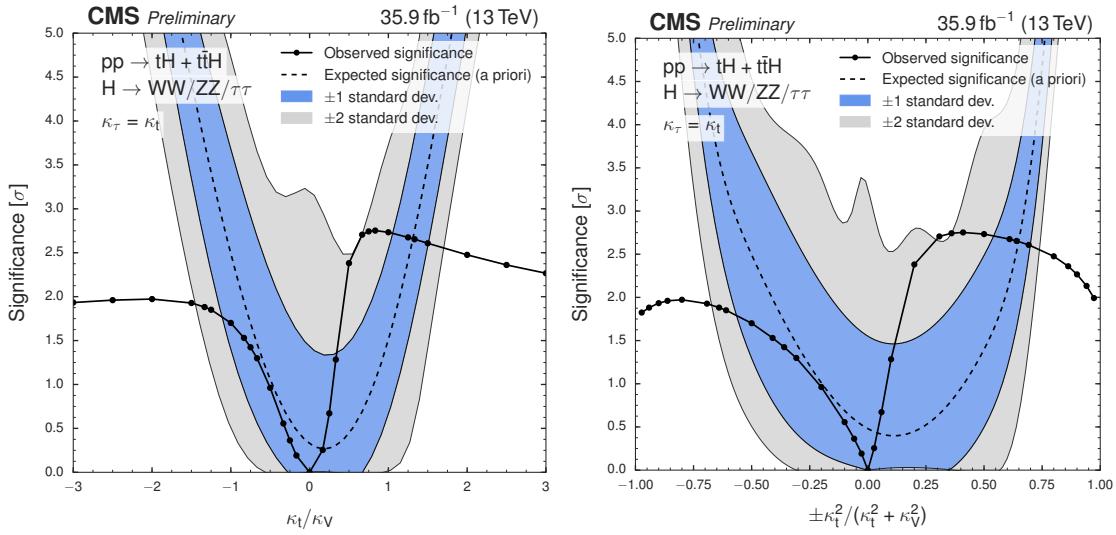
**Table 6.23:** Best fit for signal strength  $r$  and corresponding best fit cross section for the combined  $tH + t\bar{t}H$  cross section times modified branching ratio for the combination of all three channels, for the ITC and the SM-like scenarios.

$\ell\ell\ell$	$r = 1.44^{+0.91}_{-0.84}$
$e^\pm \mu^\pm$	$r = 1.42^{+1.06}_{-1.03}$
$\mu^\pm \mu^\pm$	$r = 2.75^{+1.22}_{-1.11}$
Combined	$r = 1.82^{+0.76}_{-0.69}$
Expected	$r = 1.00^{+0.70}_{-0.65}$

**Table 6.24:** Best-fit signal strengths for a SM-like Higgs signal for the individual channels.

3250 In the SM scenario, a signal strength of 1.82 is obtained which corresponds to a  
 3251 cross section of 0.33 pb. The observed significance of the signal, in a background-  
 3252 only hypothesis, is  $2.7\sigma$ , with an a-priori expected significance of  $1.5\sigma$ . For the  
 3253 ITC scenario, the best fit signal strength is 0.68, corresponding to a significance

of  $1.7\sigma$ ( $2.5\sigma$  expected); a scan of the observed and expected significances over the  $\kappa_t/\kappa_V$  configurations is shown in Fig. 6.36. Note that the fit favors a signal strength compatible with zero for a scenario with  $\kappa_t = 0$  (where the  $t\bar{t}H$  component vanishes).

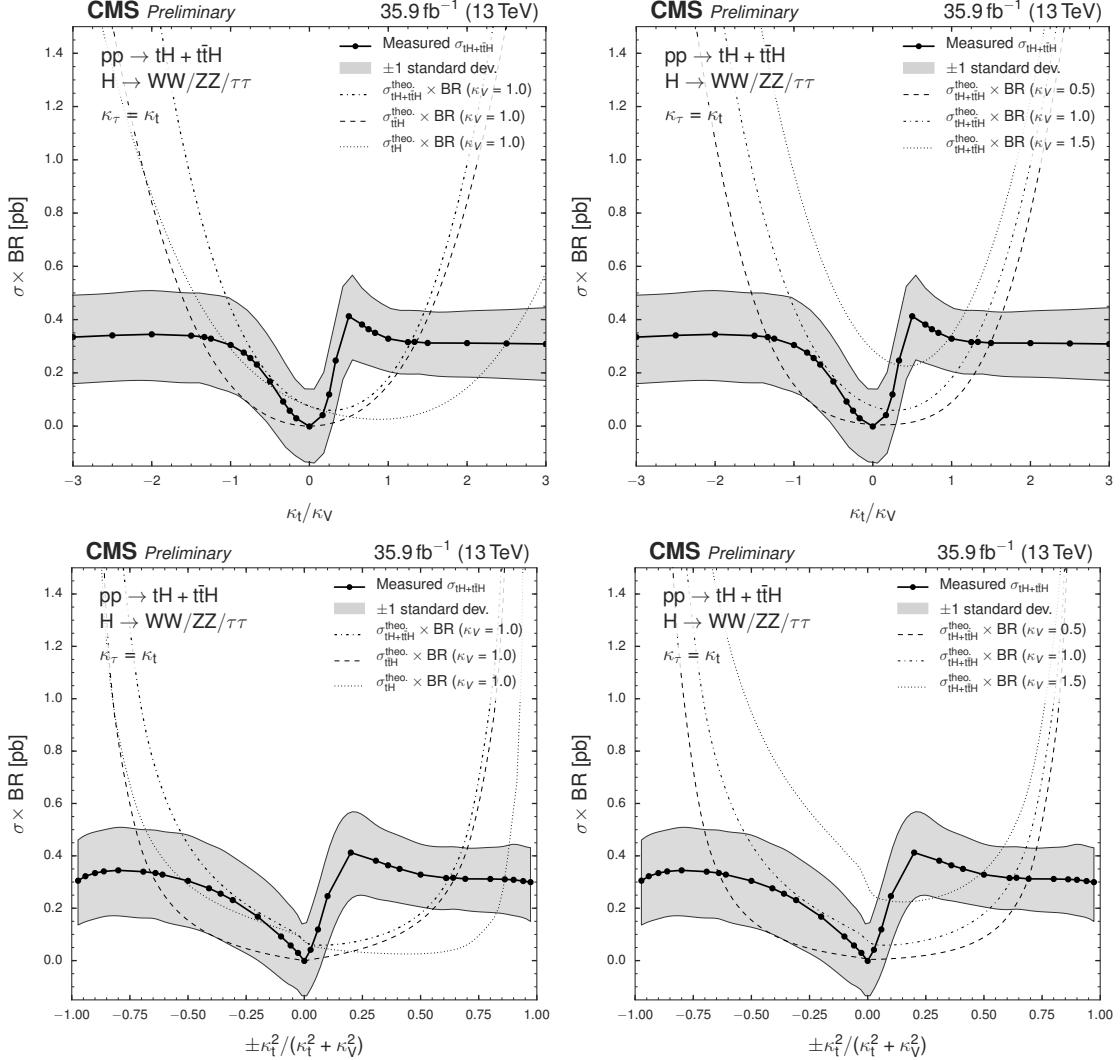


**Figure 6.36:** Observed and a priori expected significance of the fit result (in a background-only hypothesis) as a function of  $\kappa_t/\kappa_V$  (top) and  $f_t$  (bottom) for the combination of three lepton channel,  $\mu^\pm\mu^\pm$ , and  $e^\pm\mu^\pm$  channel.

A scan over the best fit values of the combined cross section times modified BR is shown in Figure 6.37. The fact that the best fit signal strength at  $\kappa_t = 0$ , where the  $t\bar{t}H$  component of the signal is zero, is compatible with zero implies that the best fit for the cross section is also compatible with zero, which again reveals that the excess in the cross section limit with respect to the expectation is not  $tH$ -like but  $t\bar{t}H$ -like.

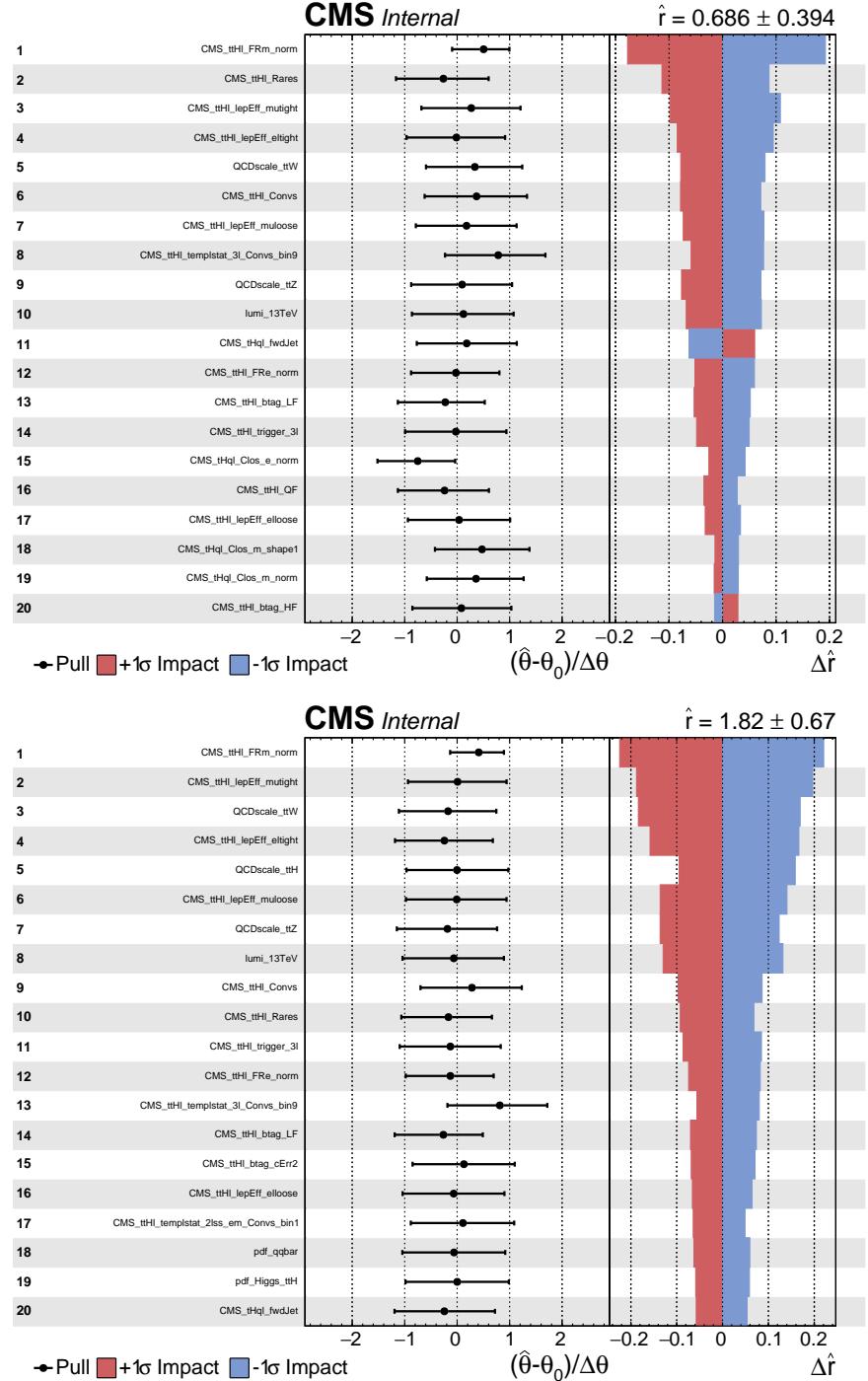
### 6.13.3 Effect of the nuisance parameters

The post-fit behavior of the most important nuisance parameters is presented in the pulls and impacts plots in Figures B.9, B.9 and B.9; additional pulls and impacts can be found in Appendix B.4

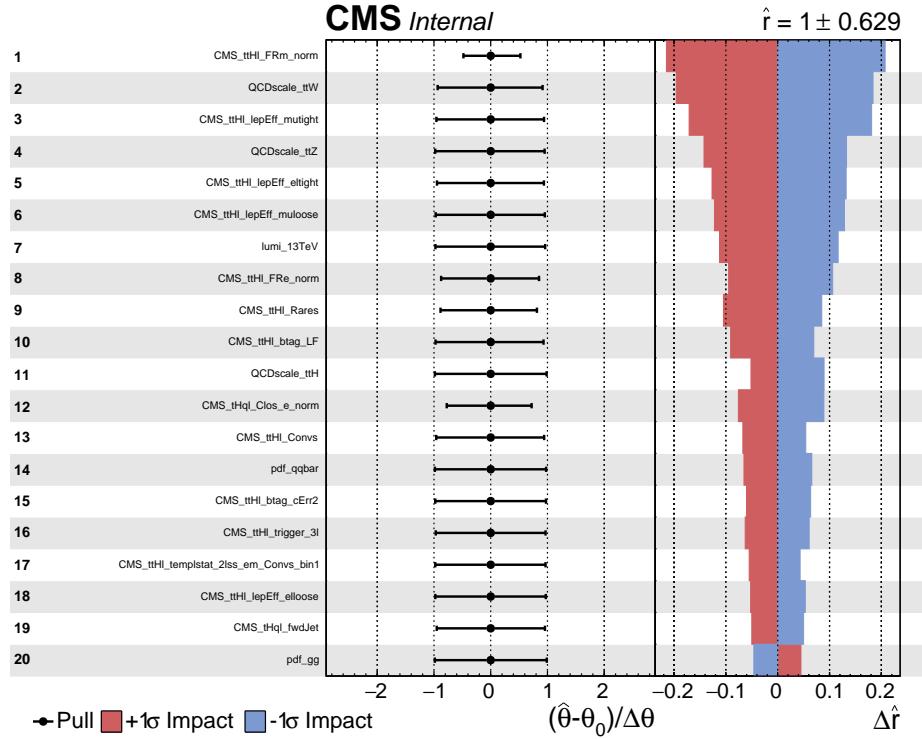


**Figure 6.37:** Best fit values of the combined  $tH + t\bar{H}$  cross section times modified BR as a function of  $\kappa_t/\kappa_V$  (top) and  $\text{sign}(\kappa_t/\kappa_V) \times \frac{\kappa_t^2}{(\kappa_t^2 + \kappa_V^2)}$  (bottom) for the combination of three lepton channel,  $\mu^\pm\mu^\pm$ , and  $e^\pm\mu^\pm$  channel.

3266        Most of the nuisance parameters stay close to their initial values. The biggest  
 3267 impact on the signal strength limits is associated to the fake rates for muons, followed  
 3268 by the lepton efficiencies and nuisances associated to the QCD scales. The lower  
 3269 impact in the ITC scenario is associated to the b-tag and  $tHq$  closure normalization  
 3270 and shape nuisances, while in the SM scenario, nuisances associated to the forward  
 3271 jet in  $tHq$  and P.D.F.s have the lower impact in the signal strength limit .



**Figure 6.38:** Post-fit pulls and impacts of the 20 nuisance parameters with largest impacts for the fit on the observed data, for the ITC (top) and SM (bottom) hypotheses.



**Figure 6.39:** Post-fit pulls and impacts of the 20 nuisance parameters with largest impacts for a fit to the Asimov dataset with fixed signal strength, for the  $\kappa_t/\kappa_V = -1.0$  hypothesis.

The sensitivity of the analysis is limited by systematic uncertainties, predominantly by those concerning the normalizations of the main background components, i.e., the non-prompt lepton estimation, the scale uncertainties for  $t\bar{t}W$  and  $t\bar{t}Z$ , as well as by the uncertainties on the measured lepton efficiency.

## 3276 6.14 CP-mixing in $tHq$

3277 The sensitivity of the  $tH$  production process to the CP-mixing in the Higgs boson  
 3278 sector was explored in Section 1.6; the theoretical model postulates the existence of a  
 3279 generic spin-0 particle  $X_0$  with CP-symmetry violating interaction with the top quark  
 3280 but SM-like interaction with the W boson.

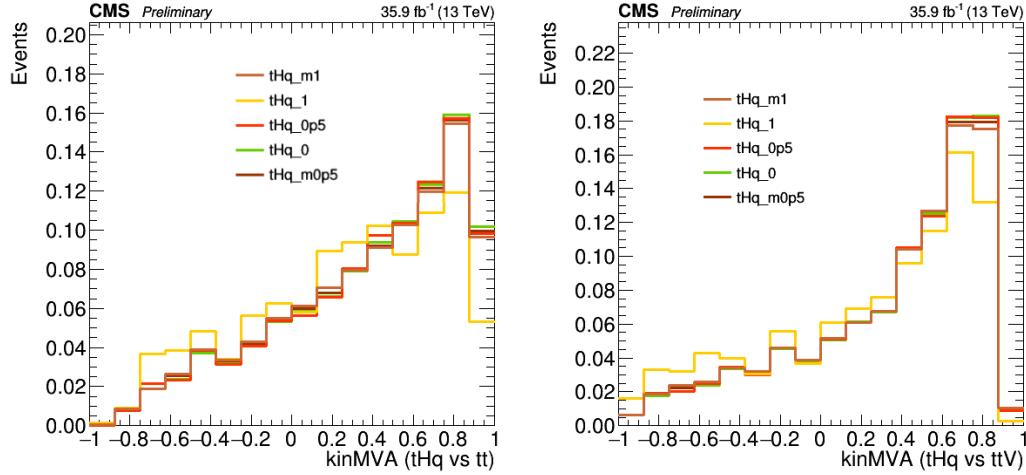
3281 The LHE reweighting procedure used in the ITC analysis is used in this CP-

$\cos(\alpha_{CP})$	Cross section (pb)		
	$tHq$	$tHW$	$t\bar{t}H$
-1.0	$0.794^{+2.8}_{-4.0}$	$0.146^{+0.2}_{-0.2}$	0.503
-0.9	$0.728^{+2.7}_{-4.1}$	$0.135^{+0.2}_{-0.2}$	0.426
-0.8	$0.664^{+2.7}_{-4.2}$	$0.123^{+0.2}_{-0.2}$	0.356
-0.7	$0.601^{+2.8}_{-4.0}$	$0.112^{+0.2}_{-0.2}$	0.296
-0.6	$0.546^{+2.9}_{-4.3}$	$0.102^{+0.2}_{-0.2}$	0.242
-0.5	$0.497^{+3.1}_{-4.2}$	$0.092^{+0.2}_{-0.2}$	0.198
-0.4	$0.446^{+3.1}_{-4.5}$	$0.083^{+0.2}_{-0.2}$	0.160
-0.3	$0.398^{+3.2}_{-4.6}$	$0.074^{+0.2}_{-0.2}$	0.132
-0.2	$0.353^{+3.5}_{-4.8}$	$0.066^{+0.2}_{-0.2}$	0.112
-0.1	$0.314^{+3.7}_{-4.9}$	$0.059^{+0.2}_{-0.2}$	0.100
0.0	$0.275^{+3.6}_{-5.2}$	$0.052^{+0.2}_{-0.2}$	0.095
0.1	$0.242^{+4.0}_{-5.5}$	$0.045^{+0.2}_{-0.2}$	0.100
0.2	$0.211^{+4.1}_{-5.8}$	$0.040^{+0.2}_{-0.2}$	0.112
0.3	$0.182^{+4.1}_{-6.1}$	$0.035^{+0.2}_{-0.2}$	0.132
0.4	$0.156^{+4.4}_{-6.5}$	$0.030^{+0.2}_{-0.2}$	0.160
0.5	$0.134^{+4.5}_{-6.6}$	$0.026^{+0.2}_{-0.2}$	0.198
0.6	$0.116^{+4.7}_{-6.9}$	$0.023^{+0.2}_{-0.2}$	0.242
0.7	$0.100^{+5.0}_{-7.1}$	$0.020^{+0.2}_{-0.2}$	0.296
0.8	$0.087^{+4.8}_{-7.1}$	$0.018^{+0.2}_{-0.2}$	0.357
0.9	$0.077^{+4.7}_{-7.0}$	$0.017^{+0.2}_{-0.2}$	0.426
1.0	$0.071^{+4.2}_{-6.7}$	$0.016^{+0.2}_{-0.2}$	0.503

**Table 6.25:** Production cross sections for  $tHq$ ,  $tHW$  and  $t\bar{t}H$  at  $\sqrt{s} = 13$  TeV, as a function of  $\cos(\alpha_{CP})$ . Uncertainties on the cross section are based on scale variations and given in %. The used  $t\bar{t}H$  NLO cross sections are provided by the authors of Reference [47] and are interpolated to the angles for which the LHE weights in the signal MC samples are available.

mixing analysis; thus, a  $tX_0q$  simulation sample was produced, containing 21 event weights for different CP-mixing angles ( $\alpha_{CP}$ ) ranging from values of  $\cos(\alpha_{CP}) = 1$  to  $\cos(\alpha_{CP}) = -1$  in steps of 0.1. The extremes of that range correspond to the previously studied points SM ( $\kappa_t = 1$ ) and the ITC ( $\kappa_t = -1$ ). The sample was produced at LO with MadGraph5\_aMCatNLO, requiring the leptonic decay of the top quark. The  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  cross sections are scaled to their NLO prediction and are listed in Table 6.25. The shape variations of the  $t\bar{t}H$  process with  $\cos(\alpha_{CP})$  are expected to be negligible in the range of values studied here where the cross section contribution is dominated by  $tH$  processes; however, the production of a private  $t\bar{t}H$

sample including the CP-mixing weights is ongoing so that they can be included in a future refinement of the analysis.

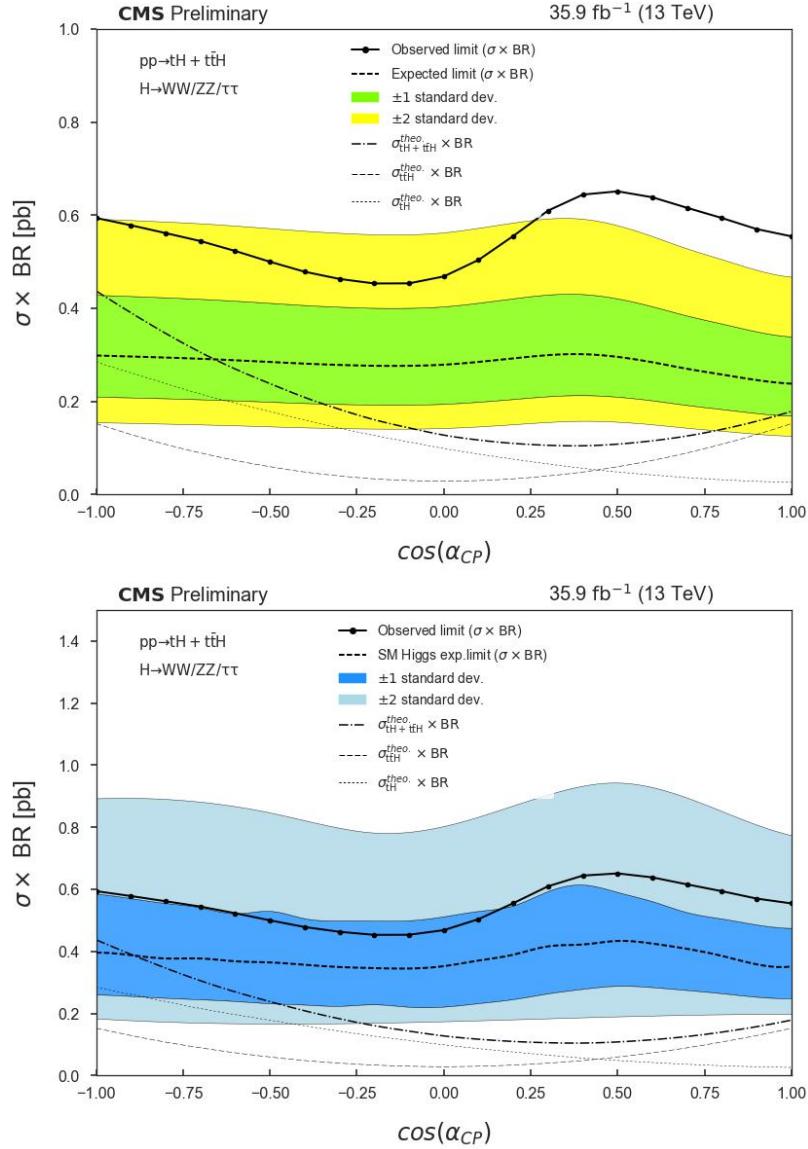


**Figure 6.40:** BDT shape variations for five CP-mixing angles. The trainings use the same set of input variables and samples as for the  $\kappa_t$ - $\kappa_V$  study. Since there are no big variations between BDT output, only one training was performed.

The set of BDTG input variables and training parameters are the same as for the  $\kappa_t$ - $\kappa_V$  analysis, as they already were optimized. Figure 6.40 shows that the shape variations for five values of  $\cos(\alpha_{CP})$ ; since there are no significant variations, it is not necessary to perform BDT trainings for each CP-mixing angle.

After performing the simultaneous fit to the observed data for all channels, the asymptotic limits are calculated for each of the CP-mixing angles. Figure 6.41 shows the expected background-only, SM-like, and observed asymptotic  $Cl_S$  limits at 95% C.L. on the combined  $tH + t\bar{t}H$  cross section times BR as a function of  $\cos(\alpha_{CP})$  for the combination of the  $3l$ ,  $\mu^\pm\mu^\pm$ , and  $e^\pm\mu^\pm$  channels for all studied CP-mixing angles; the corresponding values are listed in Table G.7. The SM-like limits and cross section limits have been calculated on an Asimov dataset that includes SM-like  $tH$  and  $t\bar{t}H$  signals.

The interpolation between estimated values was made using a cubic spline fit.



**Figure 6.41:** Left (Right): Expected background-only (SM-like including  $t\bar{t}H$  and  $tH$  signals) and observed asymptotic limits on the combined  $tH + t\bar{t}H$  cross section times BR as a function of  $\cos(\alpha_{CP})$  for the combination of three lepton channel,  $\mu^\pm\mu^\pm$ , and  $e^\pm\mu^\pm$  channel. Theoretical  $tH + t\bar{t}H$  cross section curves have been included.

3306 Table 6.26 summarizes the upper limits for the ITC ( $\cos(\alpha_{CP}) = -1$ ), SM ( $\cos(\alpha_{CP}) =$   
 3307 1), and fully pseudo-scalar ( $\cos(\alpha_{CP}) = 0$ ) CP-mixing configurations.

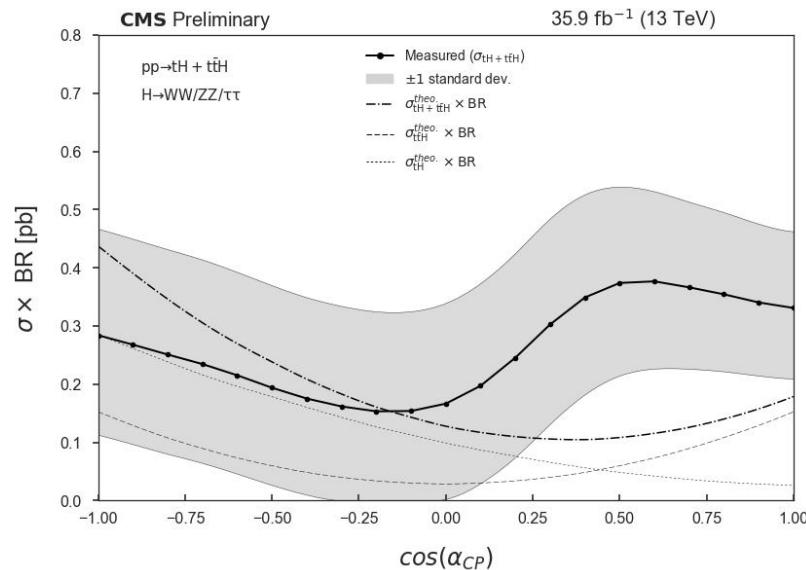
3308 The CP-mixing limits are consistent with the limits obtained in the  $\kappa_t$ - $\kappa_V$  anal-  
 3309 ysis as expected; however, in the CP-mixing case it is not possible to exclude any

Scenario	Obs. Limit	Exp. Limit		
		Median	$\pm 1\sigma$	$\pm 2\sigma$
$\cos(\alpha_{CP}) = -1$	0.594	0.299	[0.210, 0.423]	[0.155, 0.592]
$\cos(\alpha_{CP}) = 1$	0.555	0.238	[0.170, 0.340]	[0.126, 0.470]
$\cos(\alpha_{CP}) = 0$	0.469	0.279	[0.195, 0.404]	[0.143, 0.563]

**Table 6.26:** Expected (for background only) and observed 95% C.L. upper limits (in pb), for the combined  $tH + t\bar{H}$  cross section times branching ratio for the combination of all three channels, for different ITC, SM, and fully pseudo-scalar CP-mixing scenarios.

region/value in the  $\alpha_{CP}$  phase space. The excess of more than  $2\sigma$  observed in the SM scenario for the background-only expected limit, and that was also observed in the  $\kappa_t$ - $\kappa_V$  analysis, is again reduced to about  $1\sigma$  when the SM-like  $tH$  and  $t\bar{H}$  signals are included in the calculation of the expectations; however, as said above, the fact that the  $t\bar{H}$  sample does not include the CP-mixing weights implies that no conclusive sentence can be stated.

Finally, the best fit values of the combined  $tH + t\bar{H}$  cros sections times the BR as a function of the CP-mixing angle, are showed in Figure 6.42.



**Figure 6.42:** Best fit combined  $tH + t\bar{H}$   $\sigma \times BR$  as a function of the CP-mixing angle, for the combination of three lepton channel,  $\mu^\pm \mu^\pm$ , and  $e^\pm \mu^\pm$  channel. Theoretical  $tH + t\bar{H}$  cross section curves have been included.

3318 **Chapter 7**

3319 **Phase 1 FPix upgrade modules**

3320 In chapter 2, a description of the CMS pixel detector used during the collection  
3321 of the data sets used in this analysis, was presented. During the extended year-end  
3322 technical stop (EYETS) 2017, the complete CMS pixel detector was replaced in order  
3323 to support the full performance of the CMS experiment under the higher radiation  
3324 conditions produced by the increasing instantaneous luminosity delivered by the LHC  
3325 accelerator. It also was designed to address and mitigate the identified weaknesses in  
3326 the previous system.

3327 In this chapter, a description of the upgraded detector will be presented. Emphasis  
3328 will be put on the contributions made by the University of Nebraska - Lincoln (UNL)  
3329 HEP group, which consisted of the assembly of about 600 of the modules that make  
3330 up the phase 1 upgraded forward pixel detector (FPix); in particular, the gluing and  
3331 encapsulation stages will be described in detail since they are my contributions. A  
3332 complete description of the upgrade design and plans is presented in Reference [?]  
3333 which is the main source of the information contained in this section unless additional  
3334 references are provided.

## 3335 7.1 CMS pixel detector upgrade

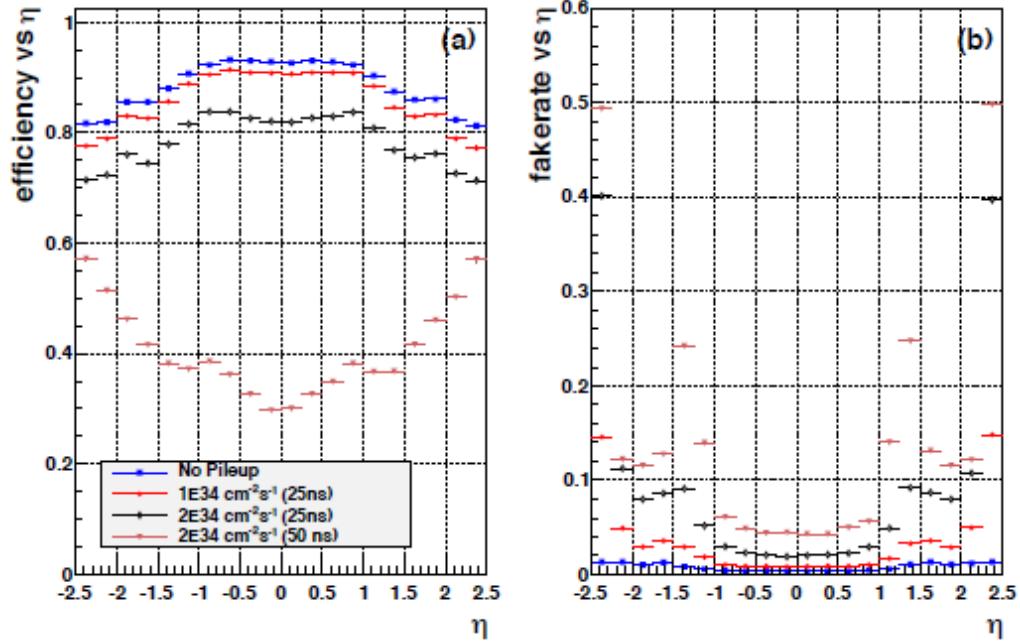
3336 The previous pixel detector was designed to record efficiently and with high precision  
 3337 the first three space-points near the interaction region, in the range of  $|\eta| < 2.5$ , at  
 3338 a instantaneous luminosity of  $1 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$  and a bunch crossing each 25 ns.  
 3339 An average pileup of about 25 simultaneous overlapping events is expected. The  
 3340 increasing luminosity would affects the performance of the detector reducing track  
 3341 reconstruction efficiency, and increasing the data loses caused by the degradation of  
 3342 the readout system; furthermore, if the LHC runs with 50 ns bunch spacing at twice  
 3343 the luminosity, then the data losses would increase almost exponentially, to losses of  
 3344 50% for the innermost layer. An illustration of the foreseen reduced performance in  
 3345 tracking efficiency and data loss is shown in Figure 7.1 in the case of simulated  $t\bar{t}$   
 3346 events at instantaneous luminosities up to  $2 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$  with 25 ns and 50 ns  
 3347 bunch spacing. The increasing fake rate is also showed. In conclusion, the prevoius  
 3348 pixel detector was not able to perform efficiently under the new luminosity, pileup,  
 3349 radiation, and running conditions.

3350 The present system is designed to offer high performance under these new oper-  
 3351 ational conditions; it is composed of four-layers/three-disks, low mass silicon pixel  
 3352 detectors providing a high performance tracking in the high luminosity environment.  
 3353 The design was leaded by the following requirements<sup>1</sup>

- 3354 • In running with 50 or more pile-up, maintain the high efficiencies and low fake  
 3355 rates.
- 3356 • New pixel readout chip (ROC) to minimize data loss due to latencies and limited  
 3357 buffering in high luminosity running.

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<sup>1</sup> Taken literally from the technical design report.



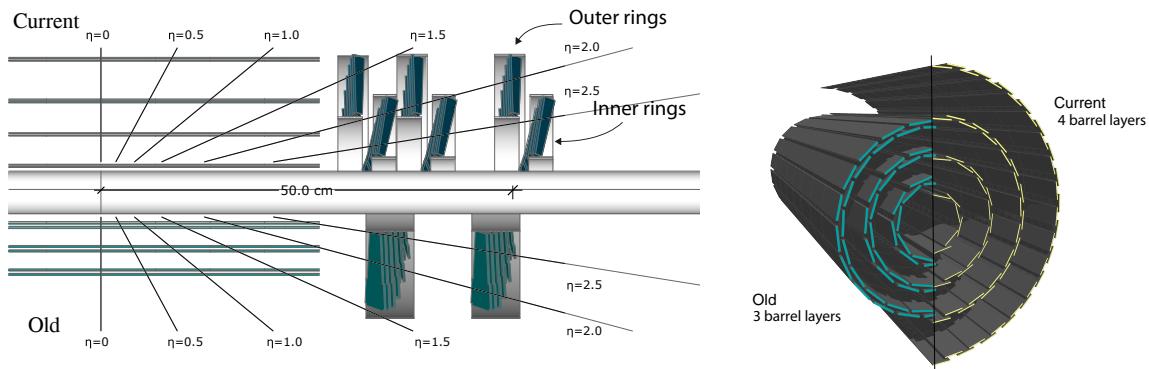
**Figure 7.1:** Expected performance of the previous pixel detector in simulated  $t\bar{t}$  events: a) efficiency; b) fake rate. Conventions are the same for both plots, considering zero pileup (blue squares), average pileup of 25 (red dots), average pileup of 50 (black diamonds), and average pileup of 100 (magenta triangles).

- 3358     • Minimize degradation due to radiation damage.
- 3359     • Optimized detector layout for 4-pixel-hit coverage over the  $\eta$  range with minimal  
3360       innermost layer radius improving pattern recognition and track reconstruction.
- 3361     • To reduce material, adopt two-phase  $CO_2$  cooling and light-weight mechani-  
3362       cal support, moving the electronic boards and connections out of the tracking  
3363       volume.
- 3364     • To reuse the current patch panel and off-detector services, cooling pipes, cables  
3365       and fibers, adopt DC-DC power converters and higher bandwidth electronics.
- 3366     • Reduce number of module types and interfaces simplifying production and main-  
3367       tenance.

3368     • New smaller diameter beam pipe to accommodate the placement of the inner  
 3369       pixel layer closer to the interaction region.

3370       The upgraded detector is expected to provide higher efficiencies, lower fake rates,  
 3371       lower dead-time/data-loss, and an extended lifetime of the detector, which translate  
 3372       in better muon ID, b-tagging, photon/electron ID, and tau reconstruction, in both  
 3373       HLT and offline levels. No details about the performance of the current pixel detector  
 3374       are given here since that matter falls beyond the purpose of this document; however,  
 3375       it is documented in Reference [159].

3376       Figure 7.2 shows the layout of the upgraded pixel detector. The old 3-layer barrel  
 3377       (BPIX), 2-disk endcap (FPix) system is replaced with a 4-layer barrel, 3-disk endcap  
 3378       system. The additional barrel layer and forward disk provide redundancy for the  
 3379       track pattern recognition and reconstruction.



**Figure 7.2:** Layout and comparison of the layers and disks in the current and old pixel detectors.

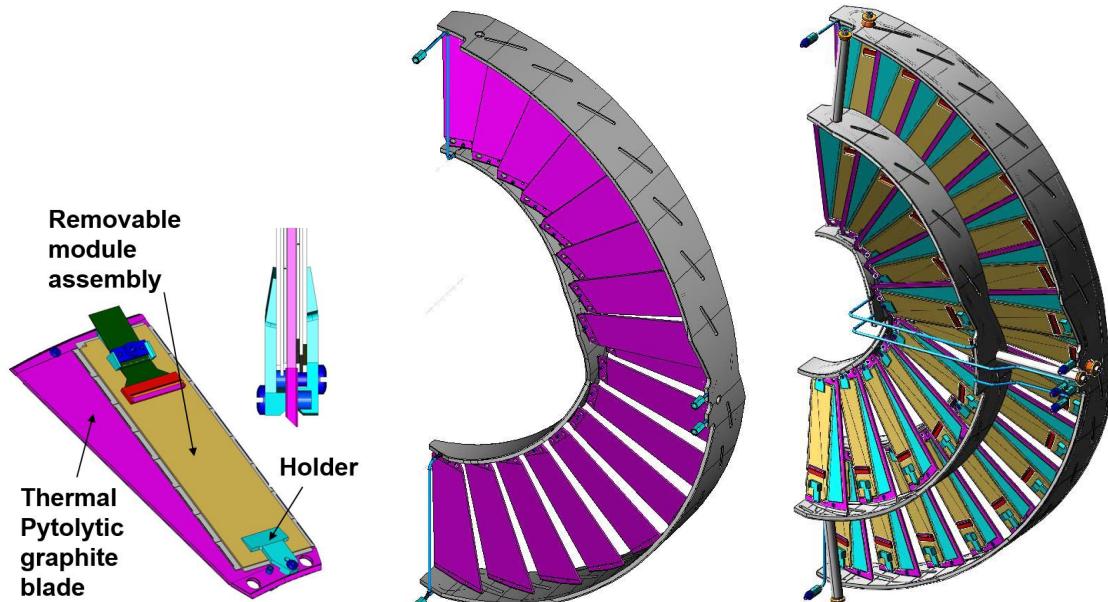
## 3380   **7.2 Phase 1 FPix upgrade**

3381       The Phase 1 upgraded FPix system is composed of three disks in each endcap, located  
 3382       at each end of the barrel detector, with a radial coverage ranging from 4.5 to 16.1

3383 cm. The first disk is located along the beam line at 29.1 cm from the IP; the second  
 3384 and third disks are located at 39.6 cm and 51.6 cm from the IP; each disk consists of  
 3385 two half disks. Some of the main features of the upgraded FPix System are:

- 3386 • Pixel size:  $100 \times 150 \mu\text{m}$
- 3387 • Only one type of modules: 2x8 ROC modules
- 3388 • Modules oriented radially to improve resolution in  $r - \phi$ .
- 3389 • Minimize the gap in 4-hit coverage between the end of the 4th-barrel layer and  
 3390 the forward-most disk.
- 3391 • All three identical disks on each side of the IP.

3392 Figure 7.3 shows a schematic structure of the FPix half disk; each half disk is  
 3393 composed of two sections, inner and outer, where the pixel modules are assembled.



**Figure 7.3:** FPix half disk design; FPix module (left) mounted on a blade, outer half disk (center), assembled half disk (right).

3394 In total, there are 56 modules (896 ROCs) per half-disk, 34 modules in the outer  
 3395 ring and 22 modules in the inner ring. The pixel modules are attached to the blades  
 3396 by a pair of module holders. Modules are designed to be removable and replace-  
 3397 able without disassembling the half-disks; thus those modules that suffer failure or  
 3398 degradation can be easily replaced during an annual technical stop.

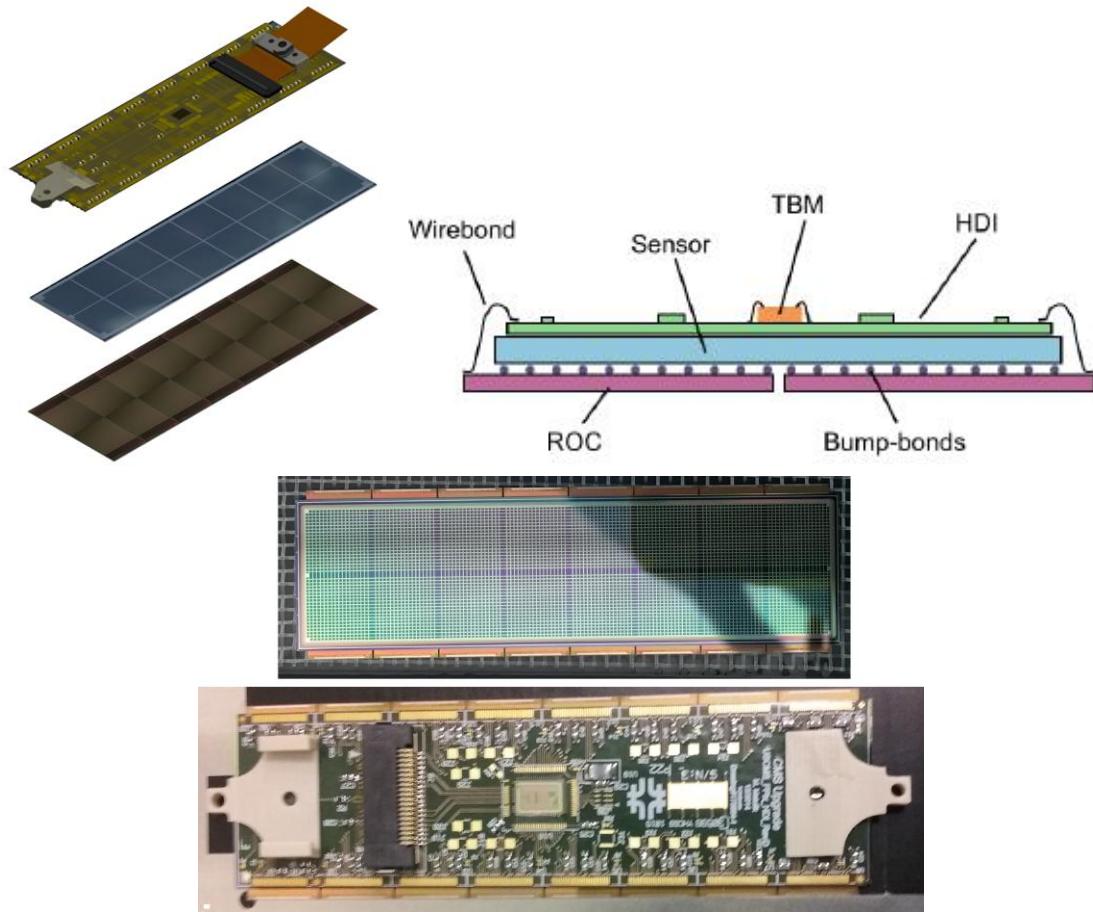
3399 Blades on the outer assembly are rotated by  $20^\circ$  forming a turbine-like geometry;  
 3400 in addition, they are arranged in an inverted cone array with the blades tilted by  $12^\circ$   
 3401 with respect to the IP in order to guarantee excellent resolution in both the azimuthal  
 3402 and radial directions throughout the FPIX acceptance angle for the inner assembly.

### 3403 7.3 FPix module structure

3404 The current CMS pixel detector is composed of 1184 pixel modules in the BPIX sector  
 3405 with a total 79 million of pixels; the FPix sector contains 672 with approximately 45  
 3406 million of pixels. Figure 7.4 shows an schematic view of the FPix modules structure.  
 3407 The  $n^+$ -in- $n$  *Silicon sensor* is Bump-Bonded to the 16 ROC to form the detector  
 3408 unit known as *Bump-Bonded Module* (BBM) with 66560 pixels. The *High Density*  
 3409 *Interconnect* (HDI) is glued on top of the BBM and wirebonded to the ROCs to  
 3410 provide them the required signals and power. The modules are attached to the  
 3411 support structure using the end holders glued to the HDI.

### 3412 7.4 FPix module assembly

3413 The construction of the modules for the current FPix system was divided between  
 3414 two sites located at Purdue University and UNL; testing facilities were located at  
 3415 University of Kansas and Fermi National Accelerator Laboratory (Fermilab). The

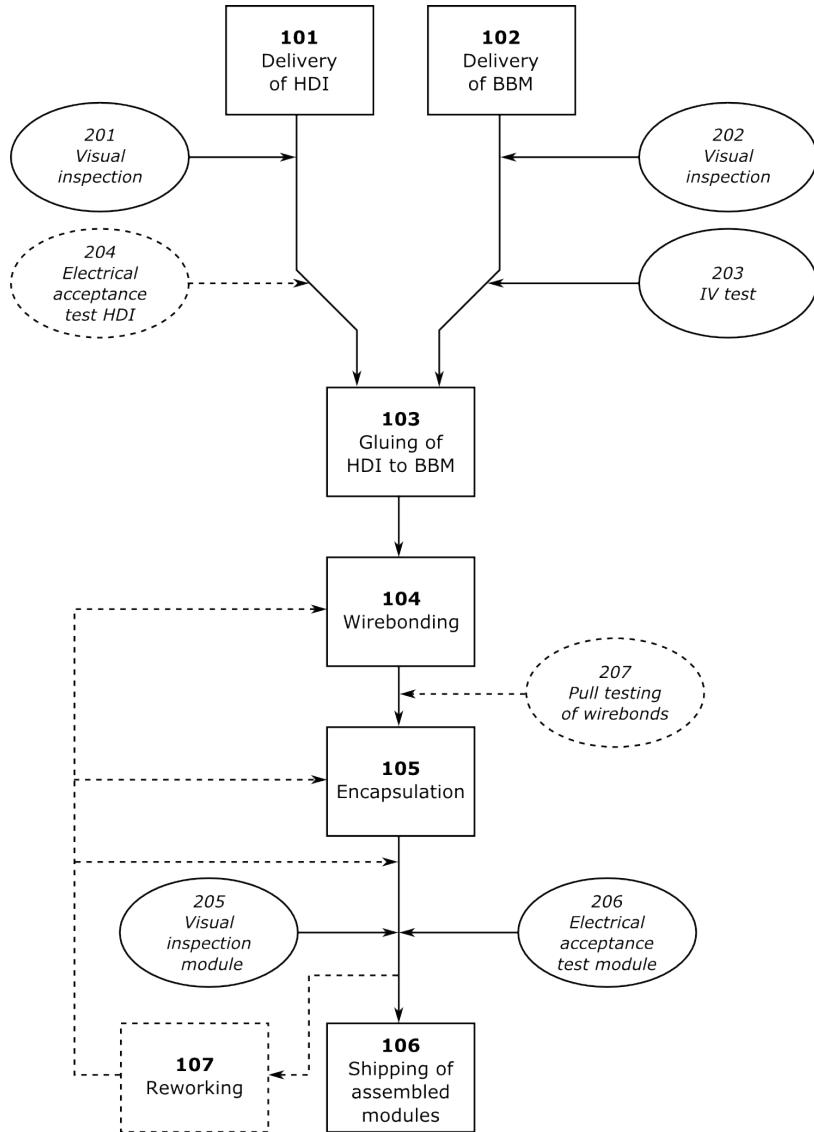


**Figure 7.4:** Top: FPix module structure; The bare silicon sensor is bump-bonded to the ROCs to form the BBM; then the HDI is glued on top of the BBM and wirebonded to the ROCs. Bottom: pictures of actual BBM and HDI.

3416 integration facility was based at Fermilab.

3417 The BBM was prepared by a commercial vendor, while the HDI was populated at  
 3418 Fermilab, with all the electronic components like resistors, capacitors and the central  
 3419 component known as *Token Bit Manager* (TBM) which is in charge of managing the  
 3420 information coming from the silicon sensors and going to the ROCs. Both BBM and  
 3421 HDI were sent to the assembly sites ready to be glued together.

3422 The module production procedure was designed following a production line struc-  
 3423 ture. Figure 7.5 shows the work flow followed at the UNL assembly site. Once the



**Figure 7.5:** UNL module assembly work flow. Dashed lines represent occasional quality testing and reworking procedures; 10X numbers represent the stage within the assembly procedure while 20X numbers represent testing stages along the assembly procedure.

3424 BBM and HDI arrive, they are submitted to visual inspection looking for defects,  
 3425 scratches, dents or short circuits. Modules passing the visual inspection are tested  
 3426 for electrical acceptance and performance. BBM and HDI are then glued employ-  
 3427 ing robotic pick-and-place machines that integrate optic tools, pattern recogni-  
 3428 tion algorithms, and glue dispensing; the semi-automated gluing process improves the

3429 uniformity of the technique. After 10 hours of curing, glued modules are moved to  
3430 the wirebonding station where ROCs and HDI are electrically connected employing  
3431 semi-automated ultrasonic wirebonding machines; occasionally, some of the wires are  
3432 pull tested for quality control. After this step, modules are fully functional, hence, a  
3433 basic functionality test is done at a subset of modules to control the manufacturing  
3434 process.

3435 In the next stage, the wirebonds are encapsulated with an elastomeric compound  
3436 (*Sylguard*) in order to protect them against mechanical damage and electrical shorts;  
3437 the encapsulation process is performed employing the robotic pick-and-place machine  
3438 which also integrates the encapsulant dispensing system. Once the encapsulation  
3439 ends, modules are mounted on module holders and submitted to a head cycle to cure  
3440 the sylguard.

3441 The module assembly sites were also responsible for the testing and characteriza-  
3442 tion of the assembled pixel modules. That testing included, visual inspection, elec-  
3443 trical acceptance, performance testing under controlled temperature conditions that  
3444 simulate the expected operational conditions; in case of any necessary reworking, the  
3445 modules were returned to the appropriate stage.

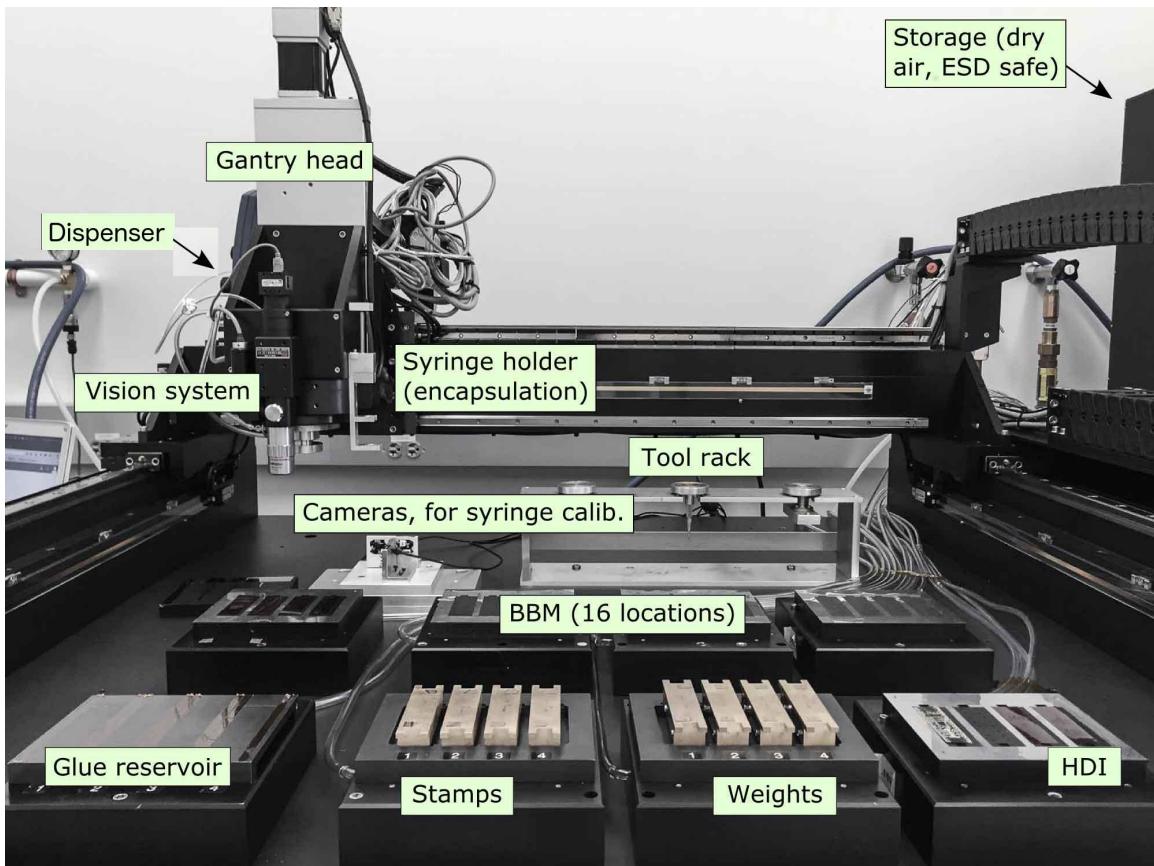
3446 In the final stage, the assembled and tested modules were shipped to University  
3447 of Kansas for further characterization.

3448 Each stage in the assembly procedure is documented with an *Standard Operat-*  
3449 *ing Procedure* (SOP) document that describes the procedures to be followed by the  
3450 operator. The full set of SOPs can be found in Reference [160].

3451 In the following sections a detailed description of the gluing and encapsulation  
3452 stages will be presented.

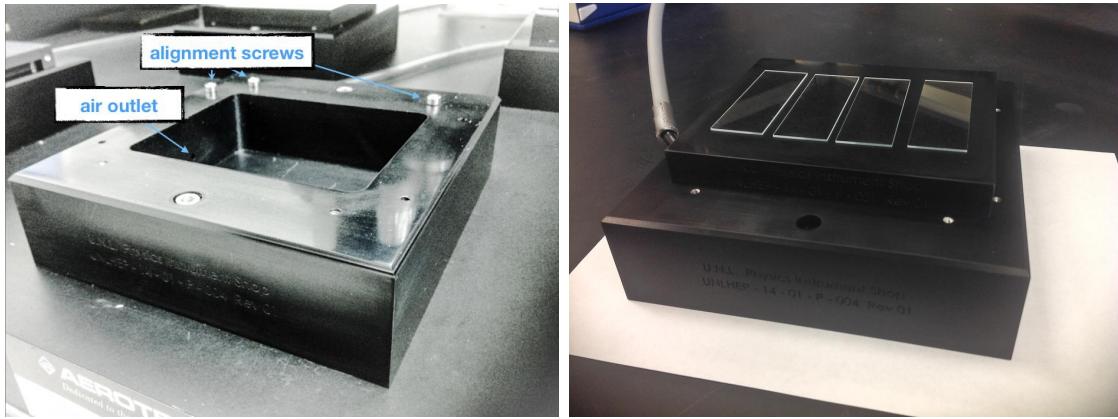
### 3453 7.4.1 Pick and place machine setup

3454 Figure 7.6 shows the full setup used to perform the gluing and encapsulation steps.  
 3455 The gantry used in the setup is a custom made *AGS15000 Series Gantry*, fabricated  
 3456 by Aerotech [161], which offers translational motion in 3D ensuring coverage of any  
 3457 position in the work field; in addition, rotational motion is provided in the *gantry*  
 3458 *head* in the usual x-y plane (gantry table plane).



**Figure 7.6:** Full gluing and encapsulation setup.

3459 A set of eight hard-anodized aluminum chucks, composed of a *base chuck* and a  
 3460 *plate chuck* each, henceforth chuck and plate respectively, were designed to house the  
 3461 parts and tools needed along the gluing process; Figure 7.7 shows the details of a  
 3462 chuck.



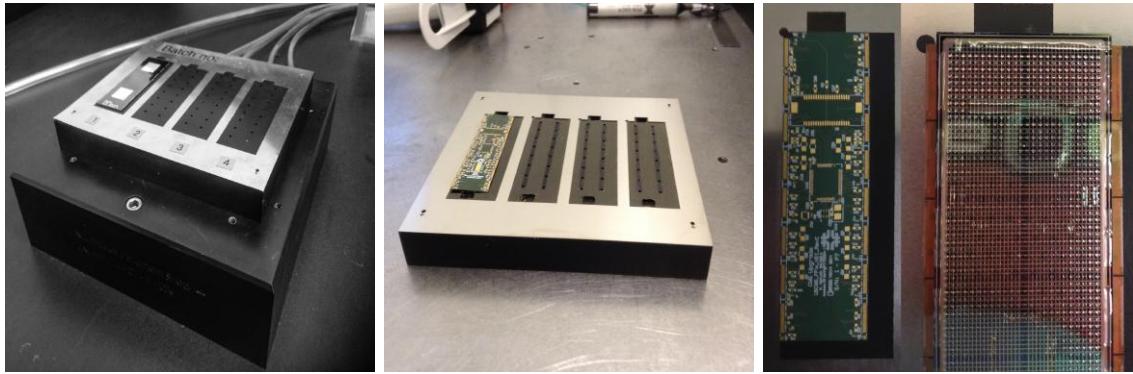
**Figure 7.7:** Left: Chuck detailed internal view. Right: full chuck housing glass slides. The vacuum connection is visible on the left.

3463        Each chuck is connected to an independent vacuum line such that the plate is  
 3464   hold fixed; both pieces are polished to seal the vacuum with no use of O-rings. The  
 3465   three screws serves as references for aligning the plates with the chucks. There are  
 3466   four types of plates; HDI/BBM plate, the glue reservoir plate, stamp plate, weight  
 3467   plate.

### 3468    Chucks

3469   Four chucks are used to accommodate sixteen BBMs (four per plate); the holes in  
 3470   the BBM/HDI plate (see Figure 7.8) are intended to hold the BBM/HDI safely fixed  
 3471   to the plate by the action of the vacuum, while the stencil (100  $\mu\text{m}$  in thickness)  
 3472   allows for a very accurate positioning of the BBM/HDI; it is thin enough so that the  
 3473   alignment is controlled by the edges of the ROC and no force is applied to the sensor.

3474        One chuck is dedicated to accommodate four HDIs. Although BBM/HDI plates  
 3475   have the same design, the HDI chuck have four independent pockets instead of only  
 3476   a big one, in order to enable the release of one HDI at a time; hence, it is connected  
 3477   to 4 vacuum lines. That is not required for the BBMs because they are no moved  
 3478   from their original location. An additional adjustment was made to the HDI plate in



**Figure 7.8:** Left: BBM/HDI plate with a mock module that reproduce the BBM features. Center: the pockets in the top and bottom sides accommodate the module holders. Right: bare HDI and BBM showing the alignment provided by the stencil.

3479 response to the HDI back surface which is not totally flat but has irregularities; these  
 3480 irregularities caused vacuum leaks that were addressed by adding a kapton tape layer  
 3481 to the HDI plate, as shown in the center of Figure 7.8. The tracks ensure the vacuum  
 3482 action and the tape flexibility ensures the sealing.

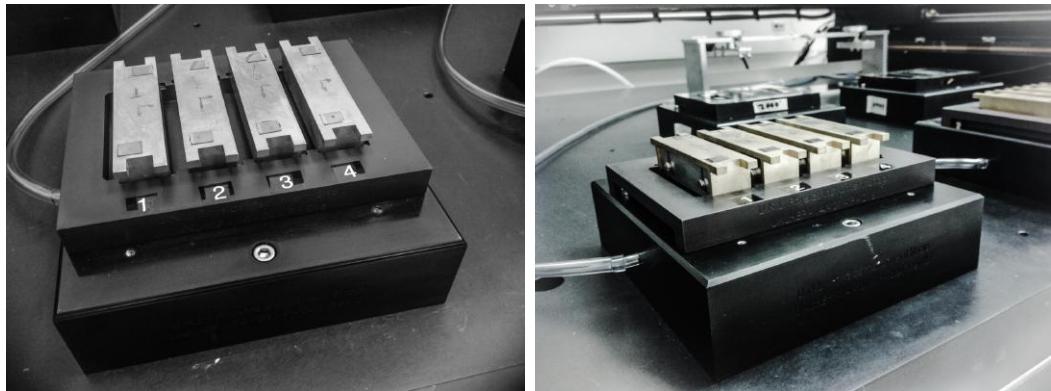
3483 One chucks holds the *glue reservoir* plate, as shown in Figure 7.9. Each of the  
 3484 four reservoirs is a pocket just 100  $\mu\text{m}$  deep, suitable for retaining sufficient glue to  
 3485 be applied to the BBM.



**Figure 7.9:** Glue reservoir plate. The four pockets are 100  $\mu\text{m}$  deep.

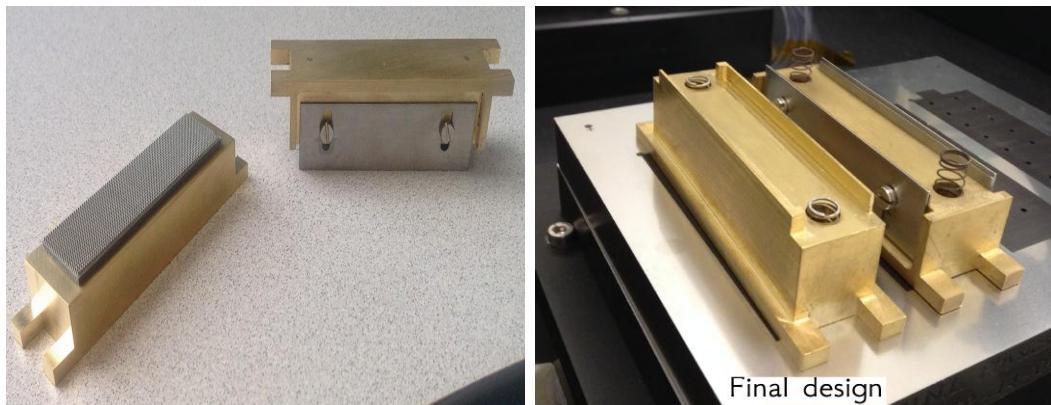
3486 The remaining two chucks house the *stamp plate* and the *weight plate* which in

3487 turn house the *stamp tools* and the *weight tools* as shown in Figure 7.10.



**Figure 7.10:** Chucks housing stamp tools(left) and weight tools(right).

3488 **Stamp and weight tools**

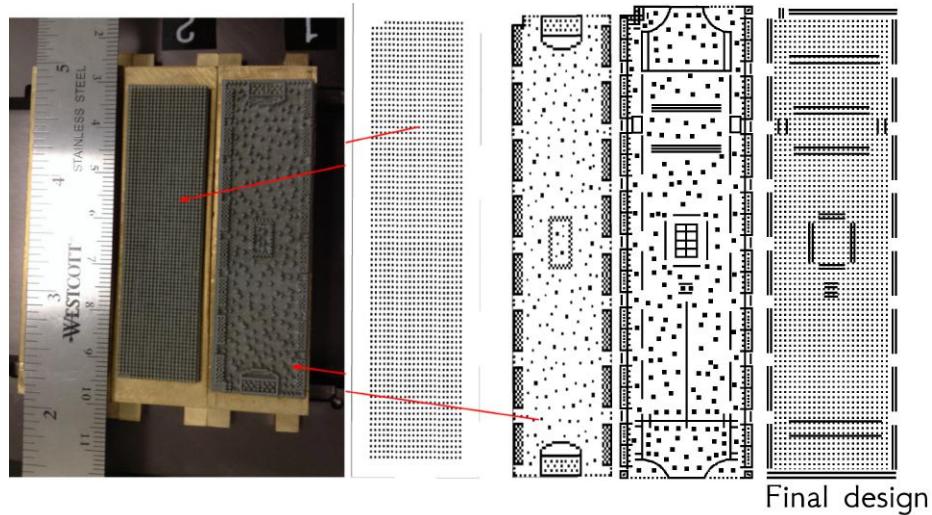


**Figure 7.11:** Stamp and weight tools. Both tools are made of brass; the stamp tool includes a rubber stamp while the weight tool includes four stainless steel blades to apply force while curing. The final weight tool design eliminates the blades (right).

3489 Stamp and weight tools are a set of custom made tools, all produced by the UNL  
 3490 Physics department machine shop (see Figure 7.11). The very first design of the  
 3491 weight tool included four stainless steel blades and two springs; the blades matched  
 3492 the rows of 8 ROC bond pads on the HDI to apply force while curing. The springs  
 3493 apply force to the module end holders on the HDI. The final design of the tool

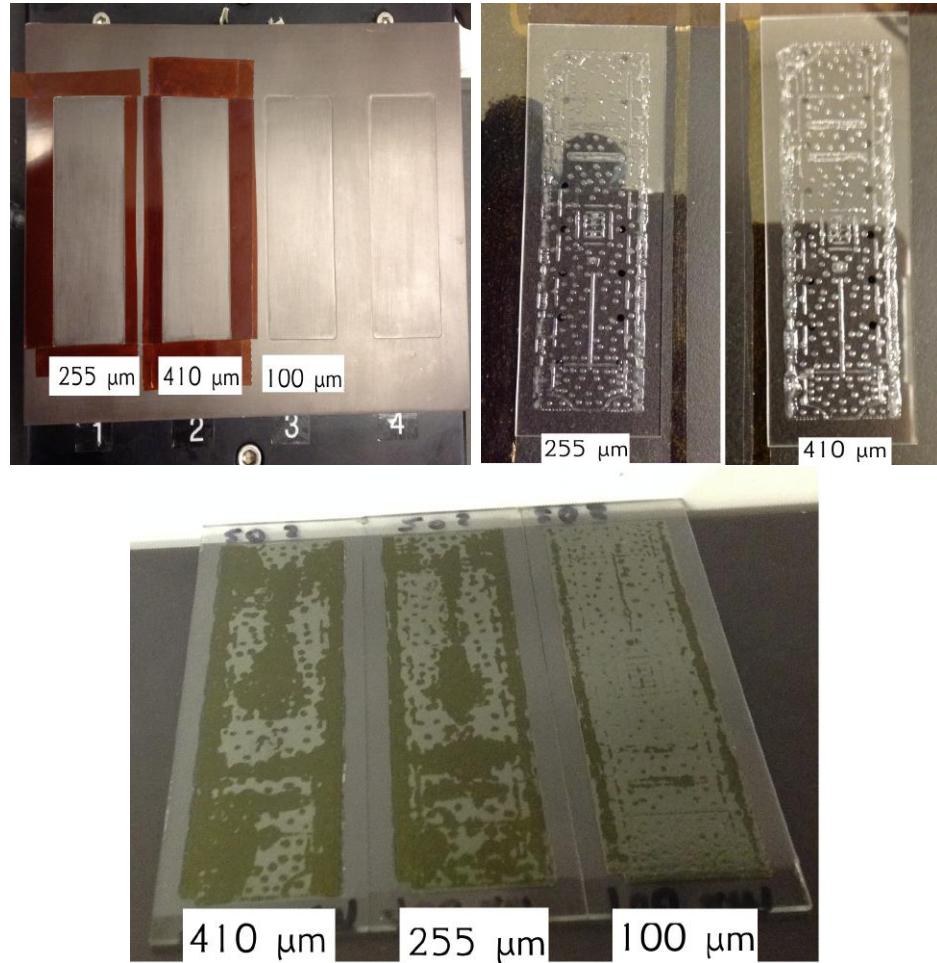
3494 eliminates the issues associated to the alignment of the blades, by integrating them  
 3495 into the design in the form of narrow blade-like brass edges. The weight tools are  
 3496 made with 260 g of brass.

3497 The stamp tool is composed of a brass piece of 200 g and a rubber stamp piece  
 3498 attached to the bottom side of the brass piece; it is used to pick the glue from the glue  
 3499 reservoir and then stamp it over the BBM. An extensive testing process was performed  
 3500 in order to determine the most appropriate features of the gluing strategy. Figure 7.12  
 3501 shows the four stamp patterns tested and a picture of the first two attached to the  
 3502 stamp tools; the variations of the stamp pattern design were based on the results  
 3503 from testing for:



**Figure 7.12:** Stamp patterns evaluated along the glue testing process; the picture on the left show the first two versions mounted on the stamp tool while the final version is on the right.

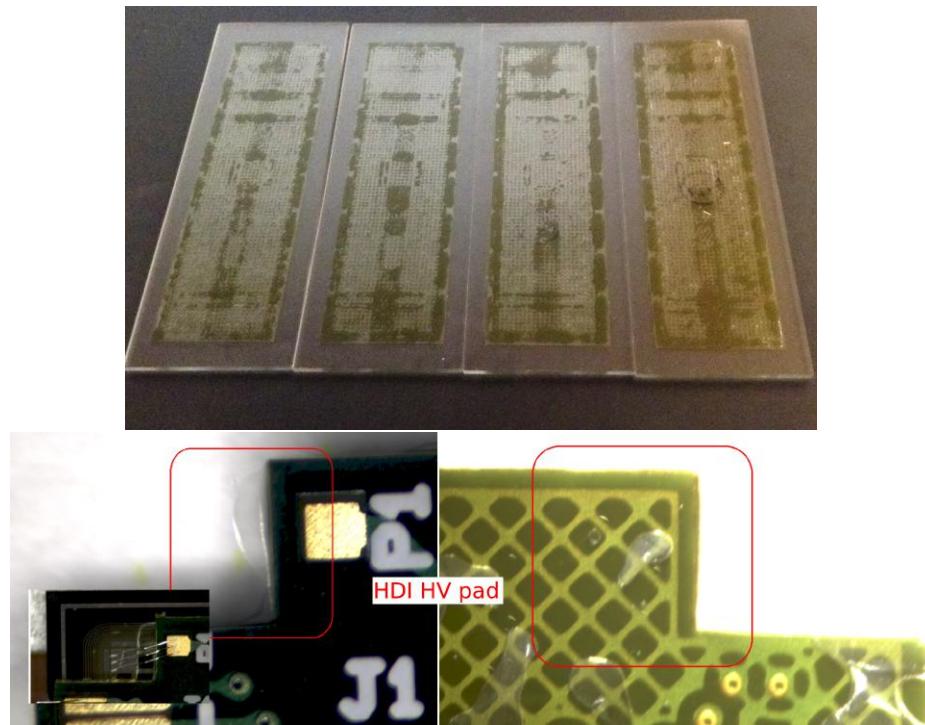
3504 • *the amount of glue dispensed*, and in particular the glue spreading out of the HDI  
 3505 area. An excess of glue, scattered beyond the HDI edge would go between the  
 3506 ROC and the sensor, affecting the functionality of the bump bonds connecting  
 3507 them; in the case of the high voltage (HV) pad, it was observed that excess of



**Figure 7.13:** Pictures of a test of the amount of glue dispensed as a function of the glue reservoir depth. The glue reservoir depth was varied by adding kapton tape (left), and the test were conducted by gluing plain HDI on top of glass slides (middle and right.)

3508       glue covered the pad on the sensor, making impossible to wire it. The amount  
 3509       of glue deposited on top of BBM depends on several variables: the dipping  
 3510       time of the stamp tool in the glue reservoir, the time that the stamp tool is in  
 3511       contact with the BBM, and the depth of the glue reservoir. In the case of the  
 3512       dipping and stamping times, it was found that there is not a strong dependence  
 3513       and those times were set to 10 seconds; in the case of the glue reservoir depth,  
 3514       the dependence is stronger. Several glue tests where conducted by gluing plain  
 3515       HDIs to glass slides; Figure 7.13 shows pictures from a glue test with three

3516 different glue reservoir depths ( $100\ \mu\text{m}$ ,  $255\ \mu\text{m}$  and  $410\ \mu\text{m}$ ). The results show  
 3517 not only that the deeper is the glue reservoir the bigger is the amount of glue  
 3518 deposited, as expected, but also that the spreading out is critical for the depths  
 3519 greater than  $200\ \mu\text{m}$ . A redesign of the rubber stamp pattern was made in  
 3520 order to reduce the amount of glue deposited in the HDI pads regions; that  
 3521 adjustment led to the final rubber stamp pattern.



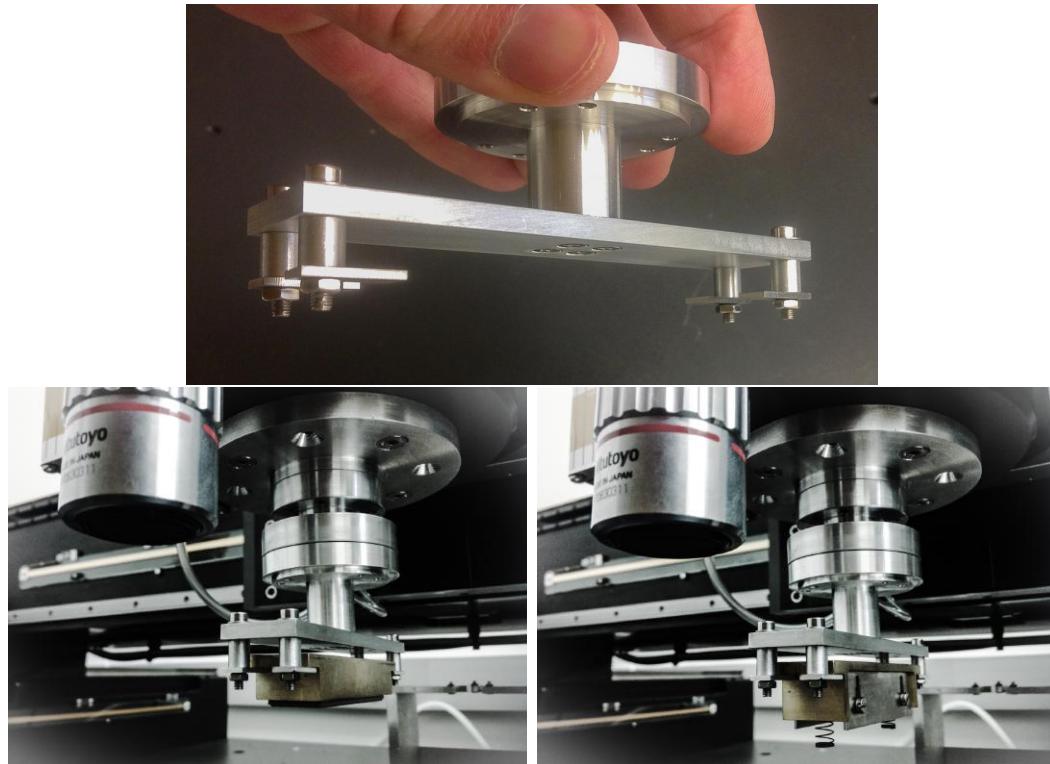
**Figure 7.14:** Results from a glue test using the final stamp pattern, which proves the support provided to the HDI bond pads and the HV pad and the almost null glue spreading out.

3522 • the size of contact area, and in particular the support given to the edges of the  
 3523 HDI where the bond pads and the HV pad are located. This is a critical aspect,  
 3524 given that the wirebonding relies on the steadiness of the pads to be connected.  
 3525 Figure 7.14 shows the outcomes of a glue test using the final stamp pattern.  
 3526 Note the support that it provides to the HDI bond pads and the HV pad and

3527 the almost null glue spreading out, which justify why it was chosen.

3528 The final tools designs used during the module production are indicated in Figures  
 3529 7.11 and 7.12, while the optimal glue reservoir depth was found to be  $100 \mu\text{m}$ .

3530 **Grabber and picker tools**

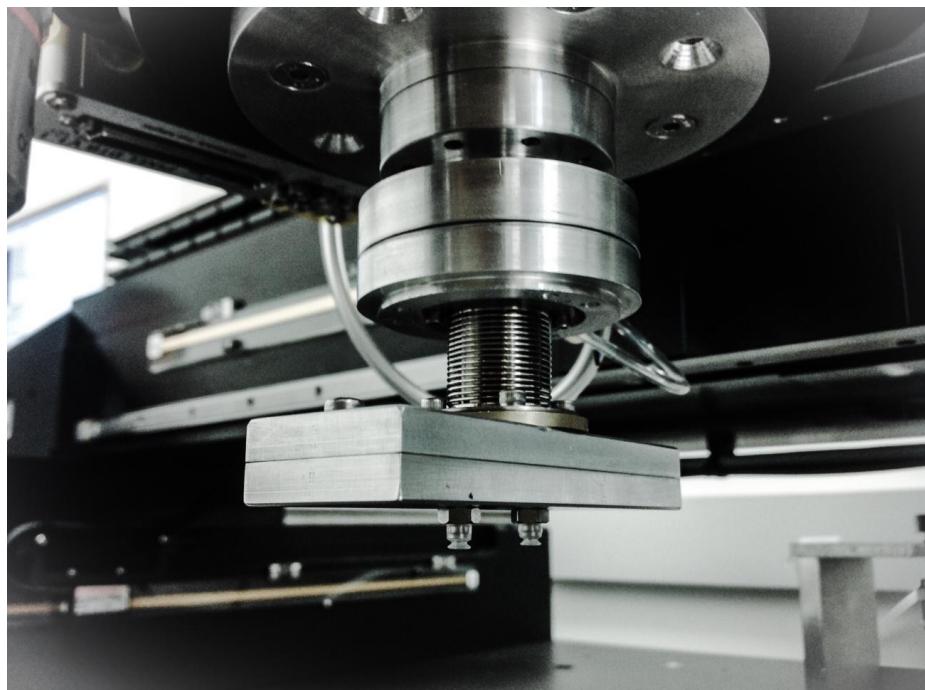


**Figure 7.15:** Top: Grabber tool used to grab the stamp and weight tools from their houses to the BBM location. Bottom: grabber tool holding the stamp (left) and weight (right) tools.

3531 In order to move the stamp and weight tools from their houses to the glue reservoir  
 3532 and to the BBM location, a *grabber tool* was designed. The grabber tool is hold on a  
 3533 tool rack located in the back of the gantry table and it gets attached to the gantry head  
 3534 by using an adapter and the vacuum system as shown in Figure 7.15. The gantry head  
 3535 adapter is attached to the rotary motor that provides the angular motion, therefore,

3536 the grabber tool is able grab the stamp and weight tools and adjust their alignment  
3537 in agreement with the BBM orientation. The force with which the glue is applied on  
3538 the BBM is controlled by the weight of the brass piece; in a similar way, the force  
3539 applied to the HDI-BBM sandwich is controlled by the weight of the tool and the  
3540 springs.

3541 The pick of the HDI and place on top of the BBM is performed using the *Picker*  
3542 *tool* showed in Figure 7.16. Same as the grabber tool, the p&p tool is hold at the  
3543 tool rack until the gantry head goes to its location and catch it using the vacuum; an  
3544 independent vacuum line is use to capture the HDI from its chuck slot. The alignment  
is performed while the HDI is being moved to the BBM location.

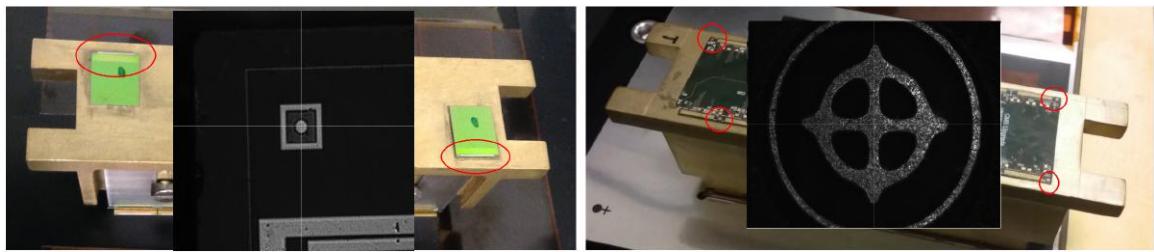


**Figure 7.16:** The pick and place tool, picks the HDI from its chuck and place it on top of the BBM.

3545

3546 **Vision system**

3547 A vision hardware system, attached to the gantry head, is used to locate the module  
 3548 components and tools employed in the assembly process. It is composed of a IDS  
 3549 HD digital camera and a Mitutoyo wide-field video microscope unit (WIDE VMU)  
 3550 as shown in Figure 7.6. The vision hardware is complemented with auto-focus and  
 3551 pattern recognition algorithms.



**Figure 7.17:** Fiducial marks attached to the stamp and weight tools. Initially, non-functional ROCs were glued on top of the tools (left) to provide the marks, located in the places indicated by red circles and showed overlapping the tool; later they were replaced by plane HDIs (right).

3552 Given that the coarse location of the HDIs, BBMs, stamp and weight tools are  
 3553 well defined by the location of the stencils and plates on the gantry table, the vision  
 3554 system is designed to search and find fiducial marks present on the materials and  
 3555 tools; these fiducial marks are placed on the HDI and BBM during their fabrication  
 3556 process. In the case of the tools, two methods were used to attach a fiducial mark  
 3557 to them: non-functional ROCs, which have on themselves fiducial marks, were glued  
 3558 on top of the tools as shown in Figure 7.17, however, during the gluing and cleaning  
 3559 processes the fiducial marks used to be covered or broken making necessary their  
 3560 replacement very often; the second method consisted of gluing plane HDIs on top of  
 3561 the tools, which not only solved the issues with the destruction of the fiducial marks  
 3562 but also simplified the pattern recognition.

3563 The procedure to find the fiducial marks starts moving the camera to an initial

3564 default calibrated position above the element, HDI, BBM or tool, such that the  
3565 image in the field of view of the camera contains the fiducial mark; then, the auto-  
3566 focus algorithm finds the best focus by measuring the contrast of pictures taken by  
3567 the camera at ten different positions in  $z$  direction around a default position where  
3568 it is assumed the best focus is; these ten contrasts are then fitted to a Gaussian  
3569 distribution where the maximum of the fitting corresponds to the best focus.

3570 Once the best focus is found, the gantry head moves the camera to that position,  
3571 takes a new picture and send it to feed the pattern recognition algorithm.

3572 The module gluing sequence begins by manually placing pre-tested, BBMs and  
3573 HDI on vacuum chucks on the baseplate of the pick-and-place machine.

3574 The machine program successively moves the camera (fixed to the machine motion  
3575 head) to view the fiducial on the BBM sensors and HDI components and acquires  
3576 the fiducial location using pattern recognition, picks up a dispensing tool from a the  
3577 tool rack and dispenses epoxy on the sensors, returns the dispensing tool to the tool  
3578 rack, picks up a vacuum tool from the tool rack to pick-and-place individual HDI  
3579 onto sensors (making adjustments based on the actual part locations in the machine  
3580 to accurately align and join the components), and returns the vacuum tool to the tool  
3581 rack. Module end holders are also aligned and glued to the modules using custom  
3582 tooling and the pick-and-place machine. Following mechanical assembly, HDI are  
3583 wirebonded to the ROCs using semi-automated ul- trasonic wirebonding machines.  
3584 Routine pull tests of sample wirebonds will be performed for quality control. The  
3585 wirebonds will be encapsulated with an elastomeric compound using semi-automated  
3586 dispensing equipment. The module assembly sites will also be responsible for the  
3587 testing and characterization of the assembled pixel modules. Modules will be ther-  
3588 mally cycled within the operating temperature range (-20  $\text{â}^{\circ}\text{C}$  to 20  $\text{â}^{\circ}\text{C}$ ) while  
3589 monitoring ROC digital and analog currents. Modules which pass the acceptance

3590 criteria will then be assembled onto the half-disk blades.

3591 The module assembly and testing schedule will depend on the throughput of the  
3592 pixel modules delivered from the bump-bonding vendors to the module assembly sites.

3593 **7.4.2 The Encapsulation stage**

3594 **7.4.3 The FPix module production yields**

<sup>3595</sup> **Appendix A**

<sup>3596</sup> **Datasets and triggers**

Dataset name
/JetHT/Run2016X-23Sep2016-vY/MINIAOD
/HTMHT/Run2016X-23Sep2016-vY/MINIAOD
/MET/Run2016X-23Sep2016-vY/MINIAOD
/SingleElectron/Run2016X-23Sep2016-vY/MINIAOD
/SingleMuon/Run2016X-23Sep2016-vY/MINIAOD
/SinglePhoton/Run2016X-23Sep2016-vY/MINIAOD
/DoubleEG/Run2016X-23Sep2016-vY/MINIAOD
/MuonEG/Run2016X-23Sep2016-vY/MINIAOD
/DoubleMuon/Run2016X-23Sep2016-vY/MINIAOD
/Tau/Run2016B-23Sep2016-v3/MINIAOD
/JetHT/Run2016H-PromptReco-v3/MINIAOD
/HTMHT/Run2016H-PromptReco-v3/MINIAOD
/MET/Run2016H-PromptReco-v3/MINIAOD
/SingleElectron/Run2016H-PromptReco-v3/MINIAOD
/SingleMuon/Run2016H-PromptReco-v3/MINIAOD
/SinglePhoton/Run2016H-PromptReco-v3/MINIAOD
/DoubleEG/Run2016H-PromptReco-v3/MINIAOD
/MuonEG/Run2016H-PromptReco-v3/MINIAOD
/DoubleMuon/Run2016H-PromptReco-v3/MINIAOD

**Table A.1:** Full 2016 dataset used in the analysis. In the first section of the table are listed the 23Sep2016 samples; in the Run2016X-23Sep-vY label, X:B-G tag the run while Y:1,3 tag the version of the data sample. Second section list the PromptReco version of the dataset.

Same-sign dilepton (==2 muons)
HLT_Mu17_TrkIsoVVL_Mu8_TrkIsoVVL_DZ_v*
HLT_Mu17_TrkIsoVVL_TkMu8_TrkIsoVVL_DZ_v*
HLT_IsoMu22_v*
HLT_IsoTkMu22_v*
HLT_IsoMu22_eta2p1_v*
HLT_IsoTkMu22_eta2p1_v*
HLT_IsoMu24_v*
HLT_IsoTkMu24_v*
Same-sign dilepton (==2 electrons)
HLT_Ele23_Ele12_CaloIdL_TrackIdL_IsoVL_DZ_v*
HLT_Ele27_eta2p1_WP Loose_Gsf_v*
HLT_Ele27_WPTight_Gsf_v*
HLT_Ele25_eta2p1_WPTight_Gsf_v*
Same-sign dilepton (==1 muon, ==1 electron)
HLT_Mu23_TrkIsoVVL_Ele8_CaloIdL_TrackIdL_IsoVL_v*
HLT_Mu8_TrkIsoVVL_Ele23_CaloIdL_TrackIdL_IsoVL_v*
HLT_Mu23_TrkIsoVVL_Ele8_CaloIdL_TrackIdL_IsoVL_DZ_v*
HLT_Mu8_TrkIsoVVL_Ele23_CaloIdL_TrackIdL_IsoVL_DZ_v*
HLT_IsoMu22_v*
HLT_IsoTkMu22_v*
HLT_IsoMu22_eta2p1_v*
HLT_IsoTkMu22_eta2p1_v*
HLT_IsoMu24_v*
HLT_IsoTkMu24_v*
HLT_Ele27_WPTight_Gsf_v*
HLT_Ele25_eta2p1_WPTight_Gsf_v*
HLT_Ele27_eta2p1_WP Loose_Gsf_v*
Three lepton
HLT_DiMu9_Ele9_CaloIdL_TrackIdL_v*
HLT_Mu8_DiEle12_CaloIdL_TrackIdL_v*
HLT_TripleMu_12_10_5_v*
HLT_Ele16_Ele12_Ele8_CaloIdL_TrackIdL_v*
HLT_Mu23_TrkIsoVVL_Ele8_CaloIdL_TrackIdL_IsoVL_v*
HLT_Mu23_TrkIsoVVL_Ele8_CaloIdL_TrackIdL_IsoVL_DZ_v*
HLT_Mu8_TrkIsoVVL_Ele23_CaloIdL_TrackIdL_IsoVL_v*
HLT_Mu8_TrkIsoVVL_Ele23_CaloIdL_TrackIdL_IsoVL_DZ_v*
HLT_Ele23_Ele12_CaloIdL_TrackIdL_IsoVL_DZ_v*
HLT_Mu17_TrkIsoVVL_Mu8_TrkIsoVVL_DZ_v*
HLT_Mu17_TrkIsoVVL_TkMu8_TrkIsoVVL_DZ_v*
HLT_IsoMu22_v*
HLT_IsoTkMu22_v*
HLT_IsoMu22_eta2p1_v*
HLT_IsoTkMu22_eta2p1_v*
HLT_IsoMu24_v*
HLT_IsoTkMu24_v*
HLT_Ele27_WPTight_Gsf_v*
HLT_Ele25_eta2p1_WPTight_Gsf_v*
HLT_Ele27_eta2p1_WP Loose_Gsf_v*

**Table A.2:** Table of high-level triggers considered in the analysis.

		<i>tHq</i>		<i>tHW</i>		
$\kappa_V$	$\kappa_t$	sum of weights	cross section [pb]	sum of weights	cross section [pb]	LHE weights
1.0	-3.0	35.700022	2.991	11.030445	0.6409	LHEweight_wgt[446]
1.0	-2.0	20.124298	1.706	5.967205	0.3458	LHEweight_wgt[447]
1.0	-1.5	14.043198	1.205	4.029093	0.2353	LHEweight_wgt[448]
1.0	-1.25	11.429338	0.9869	3.208415	0.1876	LHEweight_wgt[449]
1.0	-1.0		0.7927		0.1472	
1.0	-0.75	7.054998	0.6212	1.863811	0.1102	LHEweight_wgt[450]
1.0	-0.5	5.294518	0.4723	1.339886	0.07979	LHEweight_wgt[451]
1.0	-0.25	3.818499	0.3505	0.914880	0.05518	LHEweight_wgt[452]
1.0	0.0	2.627360	0.2482	0.588902	0.03881	LHEweight_wgt[453]
1.0	0.25	1.719841	0.1694	0.361621	0.02226	LHEweight_wgt[454]
1.0	0.5	1.097202	0.1133	0.233368	0.01444	LHEweight_wgt[455]
1.0	0.75	0.759024	0.08059	0.204034	0.01222	LHEweight_wgt[456]
1.0	1.0	0.705305	0.07096	0.273617	0.01561	LHEweight_wgt[457]
1.0	1.25	0.936047	0.0839	0.442119	0.02481	LHEweight_wgt[458]
1.0	1.5	1.451249	0.1199	0.709538	0.03935	LHEweight_wgt[459]
1.0	2.0	3.335034	0.2602	1.541132	0.08605	LHEweight_wgt[460]
1.0	3.0	10.516125	0.8210	4.391335	0.2465	LHEweight_wgt[461]
1.5	-3.0	45.281492	3.845	13.426212	0.7825	LHEweight_wgt[462]
1.5	-2.0	27.606715	2.371	7.809713	0.4574	LHEweight_wgt[463]
1.5	-1.5	20.476088	1.784	5.594971	0.3290	LHEweight_wgt[464]
1.5	-1.25	17.337465	1.518	4.635978	0.2749	LHEweight_wgt[465]
1.5	-1.0	14.483302	1.287	3.775902	0.2244	LHEweight_wgt[466]
1.5	-0.75	11.913599	1.067	3.014744	0.1799	LHEweight_wgt[467]
1.5	-0.5	9.628357	0.874	2.352505	0.1410	LHEweight_wgt[468]
1.5	-0.25	7.627574	0.702	1.789184	0.1081	LHEweight_wgt[469]
1.5	0.0	5.911882	0.5577	1.324946	0.08056	LHEweight_wgt[470]
1.5	0.25	4.479390	0.4365	0.959295	0.05893	LHEweight_wgt[471]
1.5	0.5	3.331988	0.3343	0.692727	0.04277	LHEweight_wgt[472]
1.5	0.75	2.469046	0.2558	0.525078	0.03263	LHEweight_wgt[473]
1.5	1.0	1.890565	0.2003	0.456347	0.02768	LHEweight_wgt[474]
1.5	1.25	1.596544	0.1689	0.486534	0.02864	LHEweight_wgt[475]
1.5	1.5	1.586983	0.1594	0.615638	0.03509	LHEweight_wgt[476]
1.5	2.0	2.421241	0.2105	1.170602	0.06515	LHEweight_wgt[477]
1.5	3.0	7.503280	0.5889	3.467546	0.1930	LHEweight_wgt[478]
0.5	-3.0	27.432685	2.260	8.929074	0.5136	LHEweight_wgt[479]
0.5	-2.0	13.956013	1.160	4.419093	0.2547	LHEweight_wgt[480]
0.5	-1.5	8.924438	0.7478	2.757611	0.1591	LHEweight_wgt[481]
0.5	-1.25	6.835341	0.5726	2.075247	0.1204	LHEweight_wgt[482]
0.5	-1.0	5.030704	0.4273	1.491801	0.08696	LHEweight_wgt[483]
0.5	-0.75	3.510528	0.2999	1.007273	0.05885	LHEweight_wgt[484]
0.5	-0.5	2.274811	0.1982	0.621663	0.03658	LHEweight_wgt[485]
0.5	-0.25	1.323555	0.1189	0.334972	0.01996	LHEweight_wgt[486]
0.5	0.0	0.656969	0.06223	0.147253	0.008986	LHEweight_wgt[487]
0.5	0.25	0.274423	0.02830	0.058342	0.003608	LHEweight_wgt[488]
0.5	0.5	0.176548	0.01778	0.068404	0.003902	LHEweight_wgt[489]
0.5	0.75	0.363132	0.03008	0.177385	0.009854	LHEweight_wgt[490]
0.5	1.0	0.834177	0.06550	0.385283	0.02145	LHEweight_wgt[491]
0.5	1.25	1.589682	0.1241	0.692099	0.03848	LHEweight_wgt[492]
0.5	1.5	2.629647	0.2047	1.097834	0.06136	LHEweight_wgt[493]
0.5	2.0	5.562958	0.4358	2.206057	0.1246	LHEweight_wgt[494]
0.5	3.0	14.843102	1.177	5.609519	0.3172	LHEweight_wgt[495]

**Table A.3:**  $\kappa_V$  and  $\kappa_t$  combinations generated for the two signal samples and their NLO cross sections. The *tHq* cross section is multiplied by the branching fraction of the enforced leptonic decay of the top quark (0.324) [150].

Sample	$\sigma$ [pb]
TTWJetsToLNu_TuneCUETP8M1_13TeV-amcatnloFXFX-madspin-pythia8	0.2043 *
TTZToLLNuNu_M-10_TuneCUETP8M1_13TeV-amcatnlo-pythia8	0.2529 *
/store/cmst3/group/susy/gpetrucc/13TeV/u/TTLL_m1to10_L0_NoMS_for76X/	0.0283
WGToLNuG_TuneCUETP8M1_13TeV-madgraphMLM-pythia8	585.8
ZGTo2LG_TuneCUETP8M1_13TeV-amcatnloFXFX-pythia8	131.3
TGJets_TuneCUETP8M1_13TeV_amcatnlo_madspin_pythia8	2.967
TGJets_TuneCUETP8M1_13TeV_amcatnlo_madspin_pythia8	2.967
TTGJets_TuneCUETP8M1_13TeV-amcatnloFXFX-madspin-pythia8	3.697
WpWpJJ_EWK-QCD_TuneCUETP8M1_13TeV-madgraph-pythia8	0.03711
ZZZ_TuneCUETP8M1_13TeV-amcatnlo-pythia8	0.01398
WWZ_TuneCUETP8M1_13TeV-amcatnlo-pythia8	0.1651
WZZ_TuneCUETP8M1_13TeV-amcatnlo-pythia8	0.05565
WW_DoubleScattering_13TeV-pythia8	1.64
tZq_ll_4f_13TeV-amcatnlo-pythia8_TuneCUETP8M1	0.0758
ST_tW11_5f_LO_13TeV-MadGraph-pythia8	0.01123
TTTT_TuneCUETP8M1_13TeV-amcatnlo-pythia8	0.009103
WZTo3LNu_TuneCUETP8M1_13TeV-powheg-pythia8	4.4296
ZZTo4L_13TeV_powheg_pythia8	1.256
TTJets_SingleLeptFromTbar_TuneCUETP8M1_13TeV-madgraphMLM-pythia8	182.1754 *
TTJets_SingleLeptFromT_TuneCUETP8M1_13TeV-madgraphMLM-pythia8	182.1754 *
TTJets_DiLept_TuneCUETP8M1_13TeV-madgraphMLM-pythia8	87.3 *
DYJetsToLL_M-10to50_TuneCUETP8M1_13TeV-amcatnloFXFX-pythia8	18610
DYJetsToLL_M-50_TuneCUETP8M1_13TeV-madgraphMLM-pythia8	6024
WJetsToLNu_TuneCUETP8M1_13TeV-amcatnloFXFX-pythia8	61526.7
ST_tW_top_5f_inclusiveDecays_13TeV-powheg-pythia8_TuneCUETP8M1	35.6
ST_tW_antitop_5f_inclusiveDecays_13TeV-powheg-pythia8_TuneCUETP8M1	35.6
ST_t-channel_4f_leptonDecays_13TeV-amcatnlo-pythia8_TuneCUETP8M1	70.3144
ST_t-channel_antitop_4f_leptonDecays_13TeV-powheg-pythia8_TuneCUETP8M1	26.2278
ST_s-channel_4f_leptonDecays_13TeV-amcatnlo-pythia8_TuneCUETP8M1	3.68064
WWTo2L2Nu_13TeV-powheg	10.481
ttWJets_13TeV_madgraphMLM	0.6105
ttZJets_13TeV_madgraphMLM	0.5297/0.692

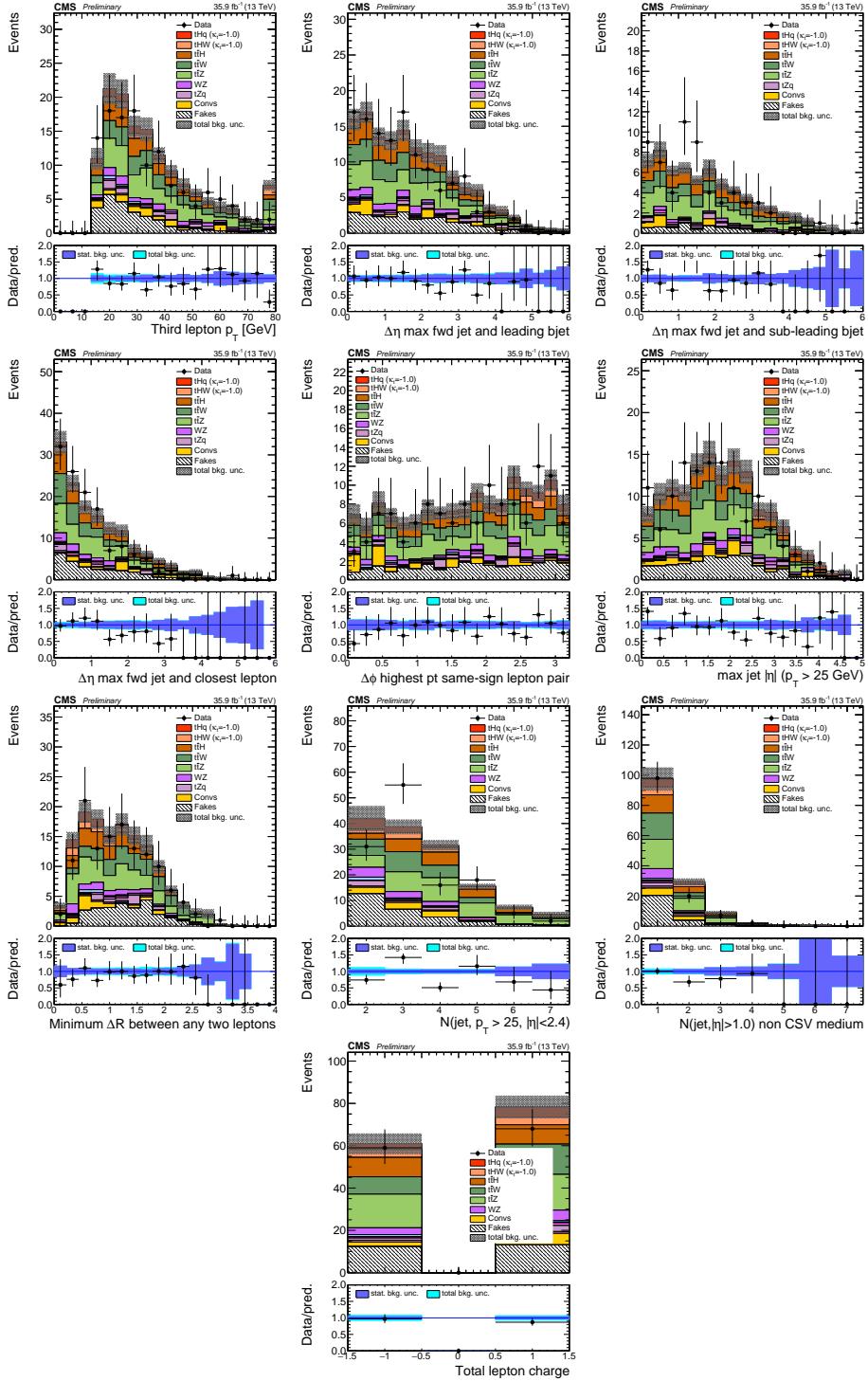
**Table A.4:** List of background samples used in this analysis (CMSSW 80X). The first section of the table lists the samples used in simulation to extract the final yields and shapes; the second section lists the samples of the processes for which the yields are estimated from data. The MC simulation is used to design the data driven methods and in the derivation of the associated systematic uncertainties. The third section list the leading order  $t\bar{t}W$  and  $t\bar{t}Z$  samples, which in addition to the ones marked with a \*, where used in the BDT training.

<sup>3597</sup> **Appendix B**

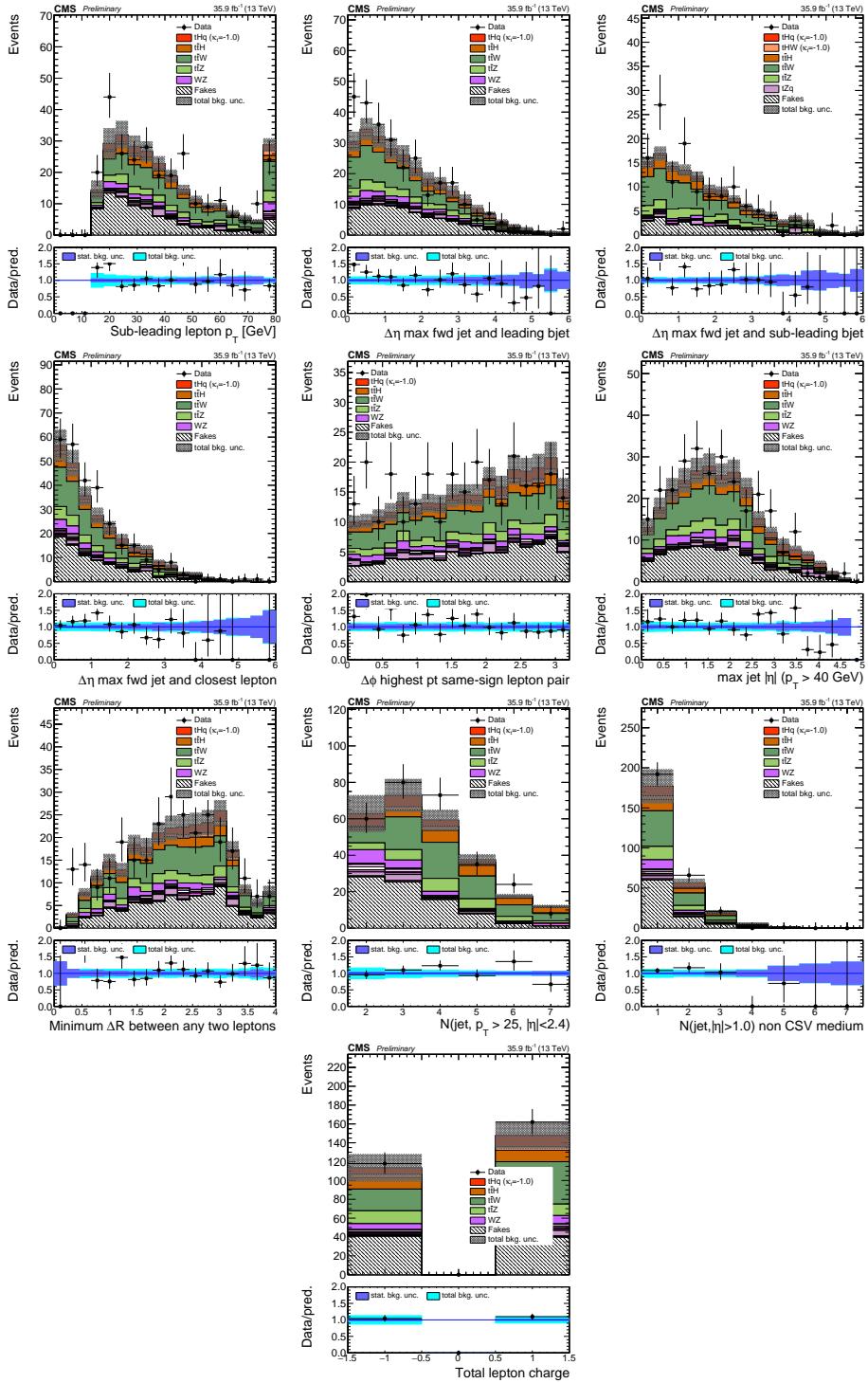
<sup>3598</sup> **Aditional plots**

<sup>3599</sup> **B.1 Pre-selection kinematic variables**

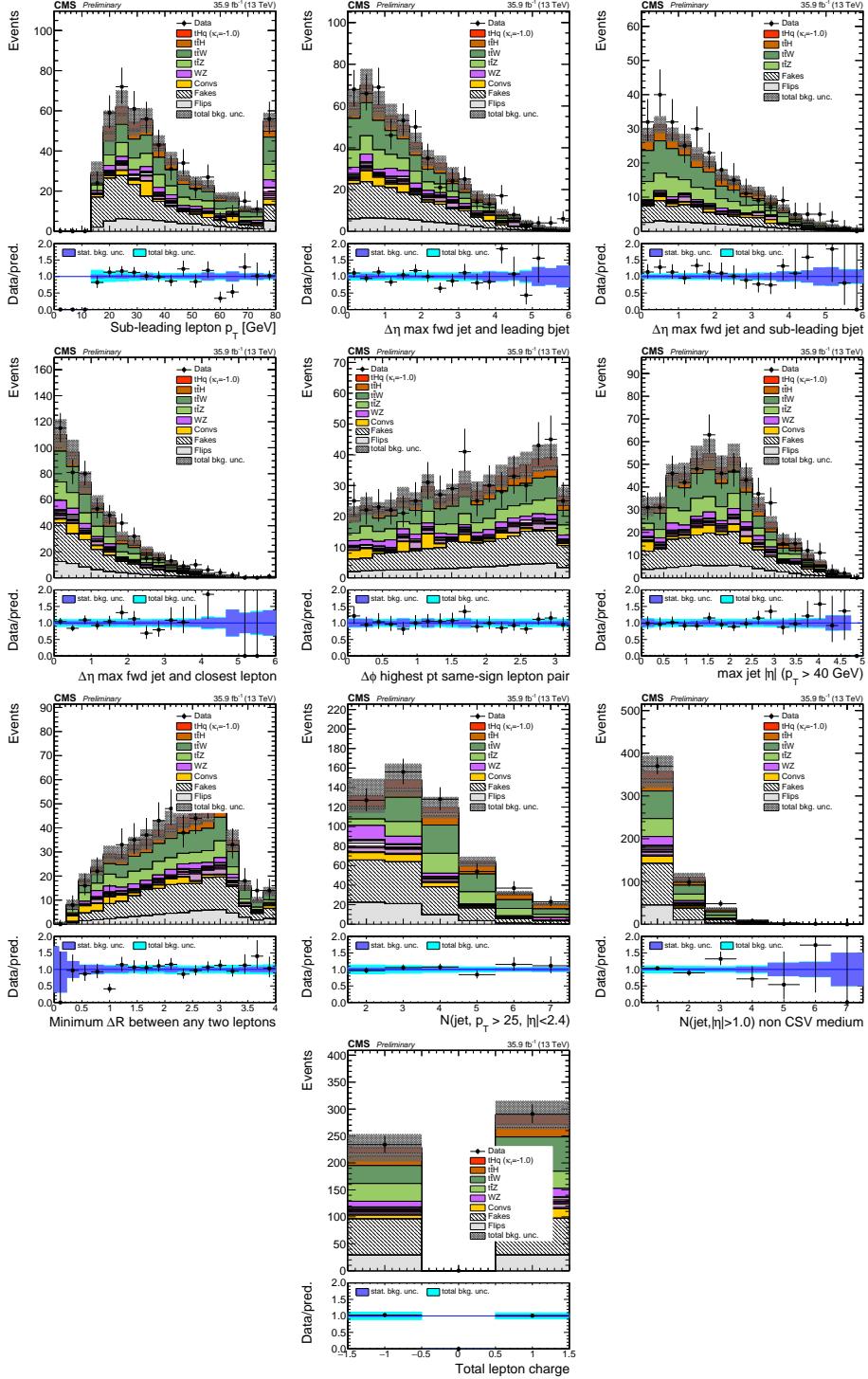
<sup>3600</sup> Figures B.1, B.2 and B.3 show the distributions of some relevant kinematic variables,  
<sup>3601</sup> normalized to the cross section of the respective processes and to the integrated  
<sup>3602</sup> luminosity.



**Figure B.1:** Distributions of input variables to the BDT for signal discrimination, three lepton channel, normalized to their cross section and to  $35.9 \text{ fb}^{-1}$ .

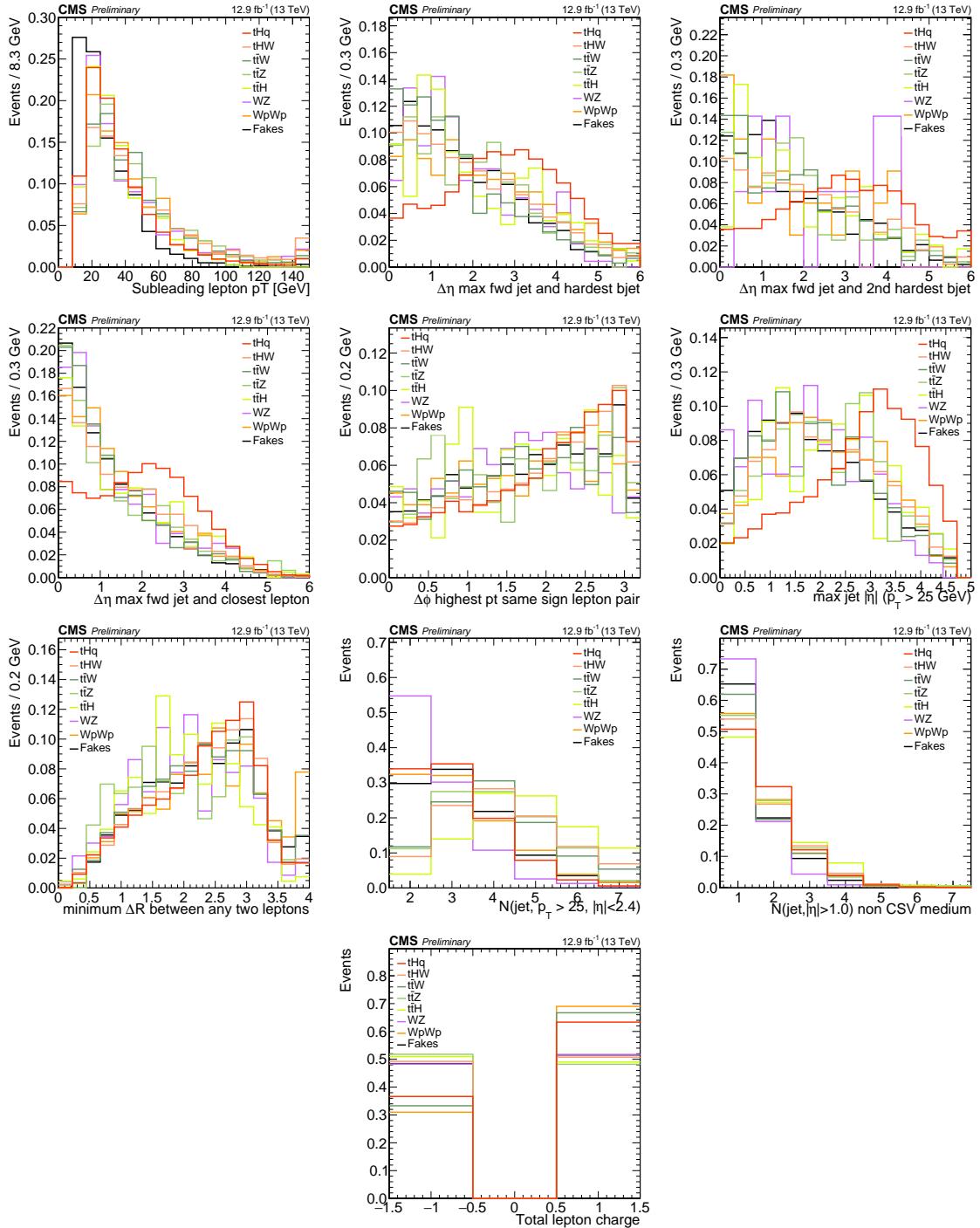


**Figure B.2:** Distributions of input variables to the BDT for signal discrimination, in  $\mu^\pm \mu^\pm$  channel, normalized to their cross section and to  $35.9 \text{ fb}^{-1}$ .



**Figure B.3:** Distributions of input variables to the BDT for signal discrimination, in  $e^\pm\mu^\pm$  channel, normalized to their cross section and to  $35.9 \text{ fb}^{-1}$ .

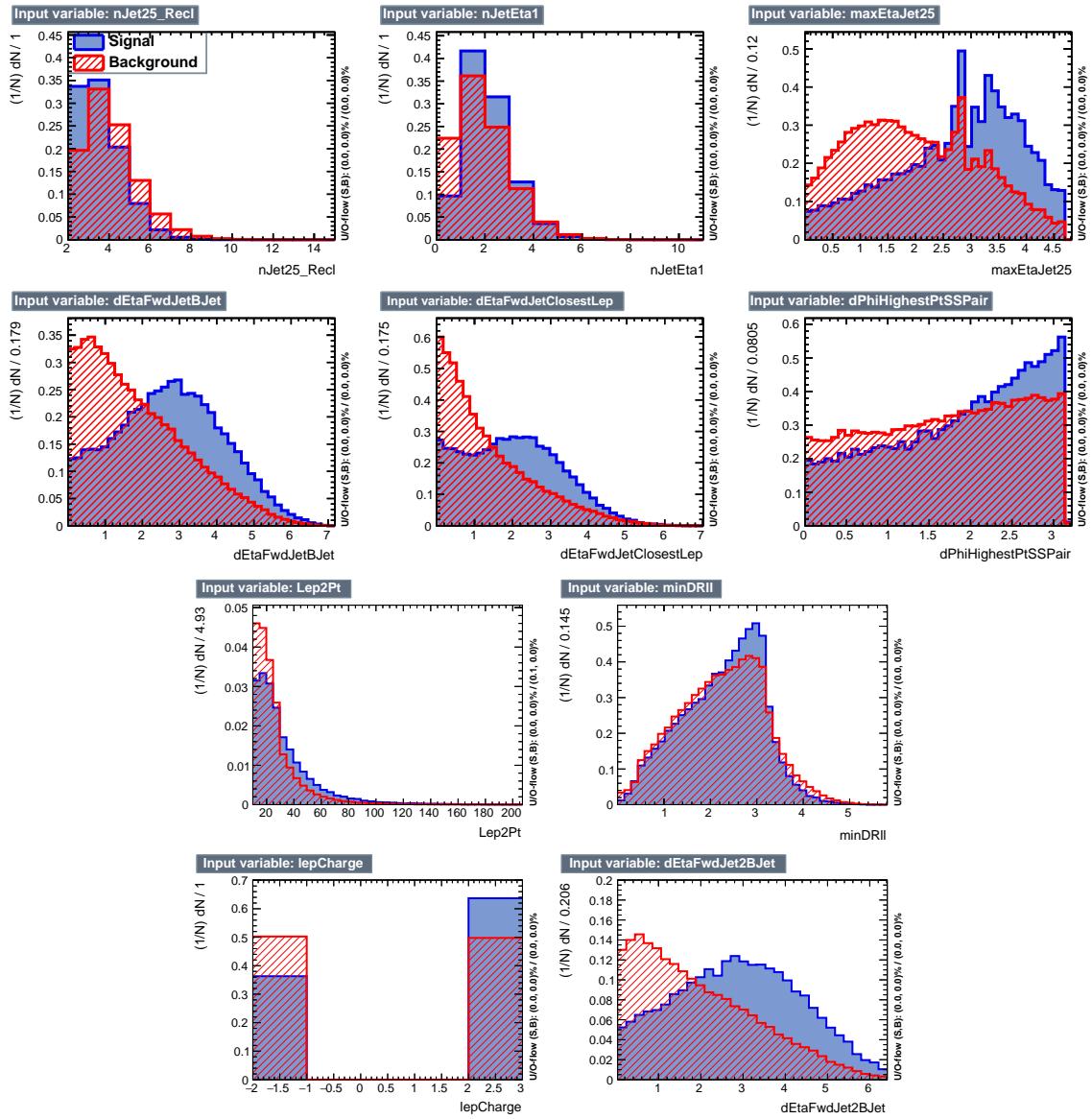
3603 B.2 BDTG input variables for  $2lss$  channel



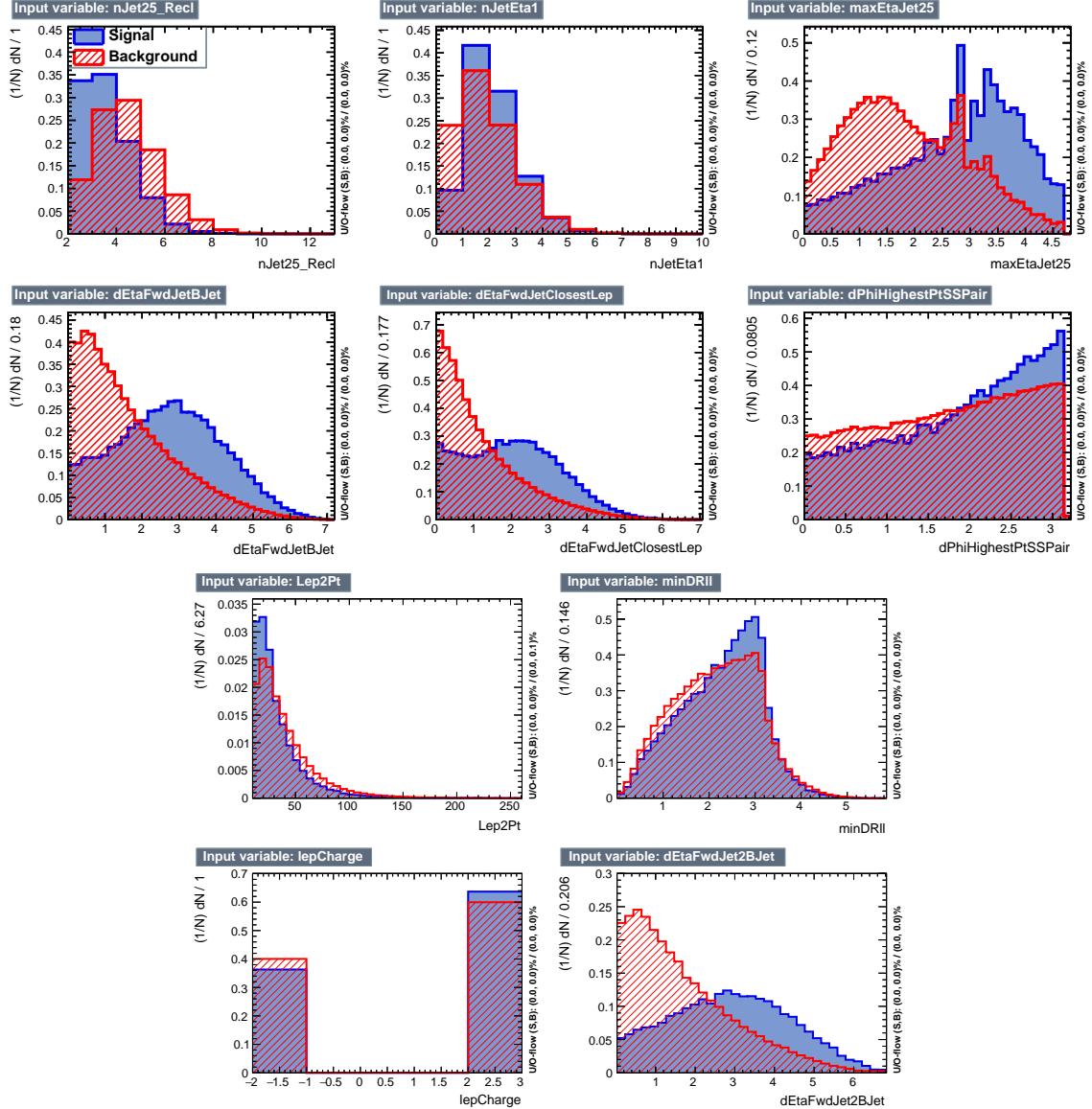
**Figure B.4:** Distributions of input variables to the BDT for signal discrimination, two lepton same sign channel.

3604    **B.3 Input variables distributions from BDTG**

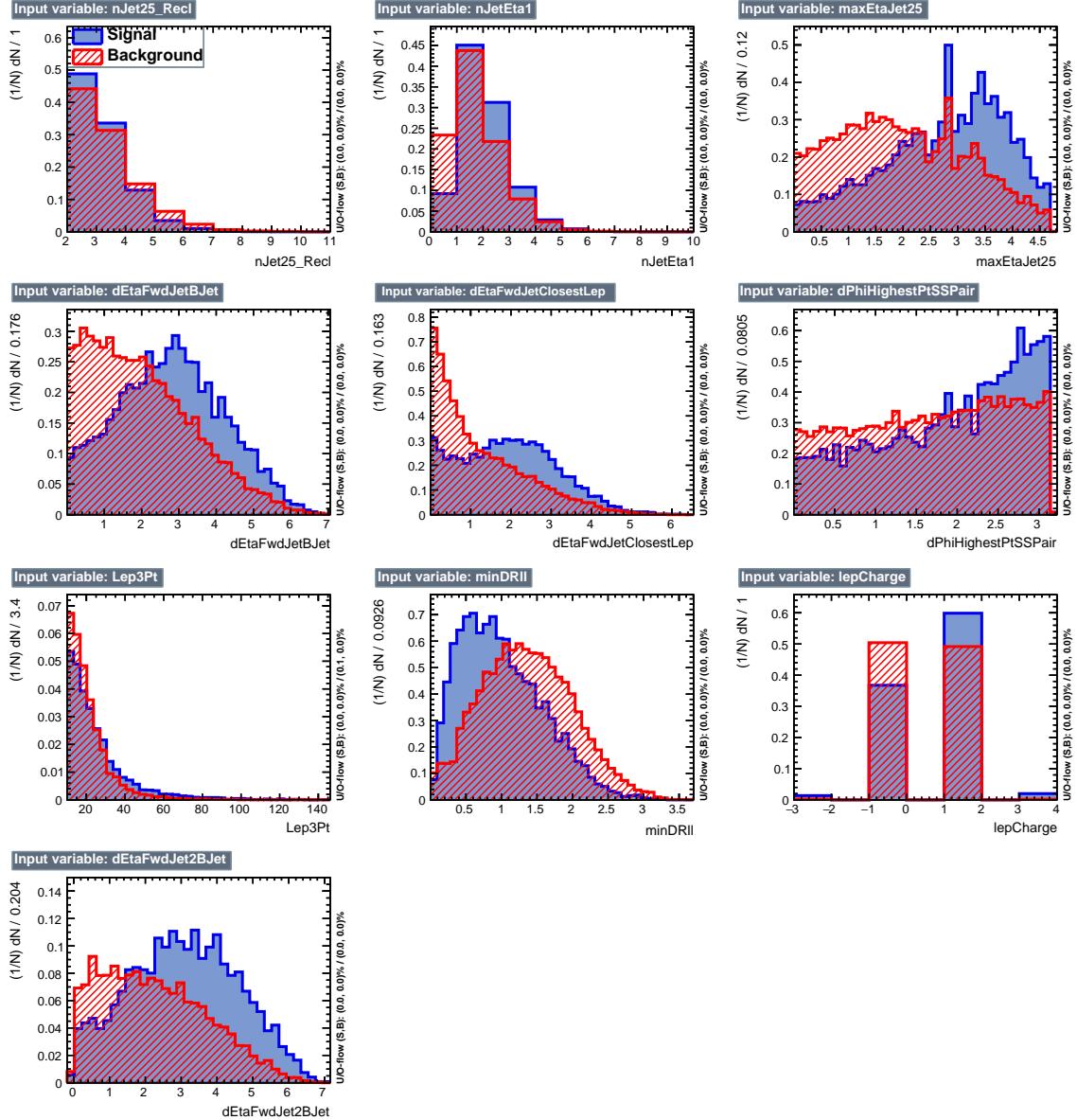
3605    classifiers



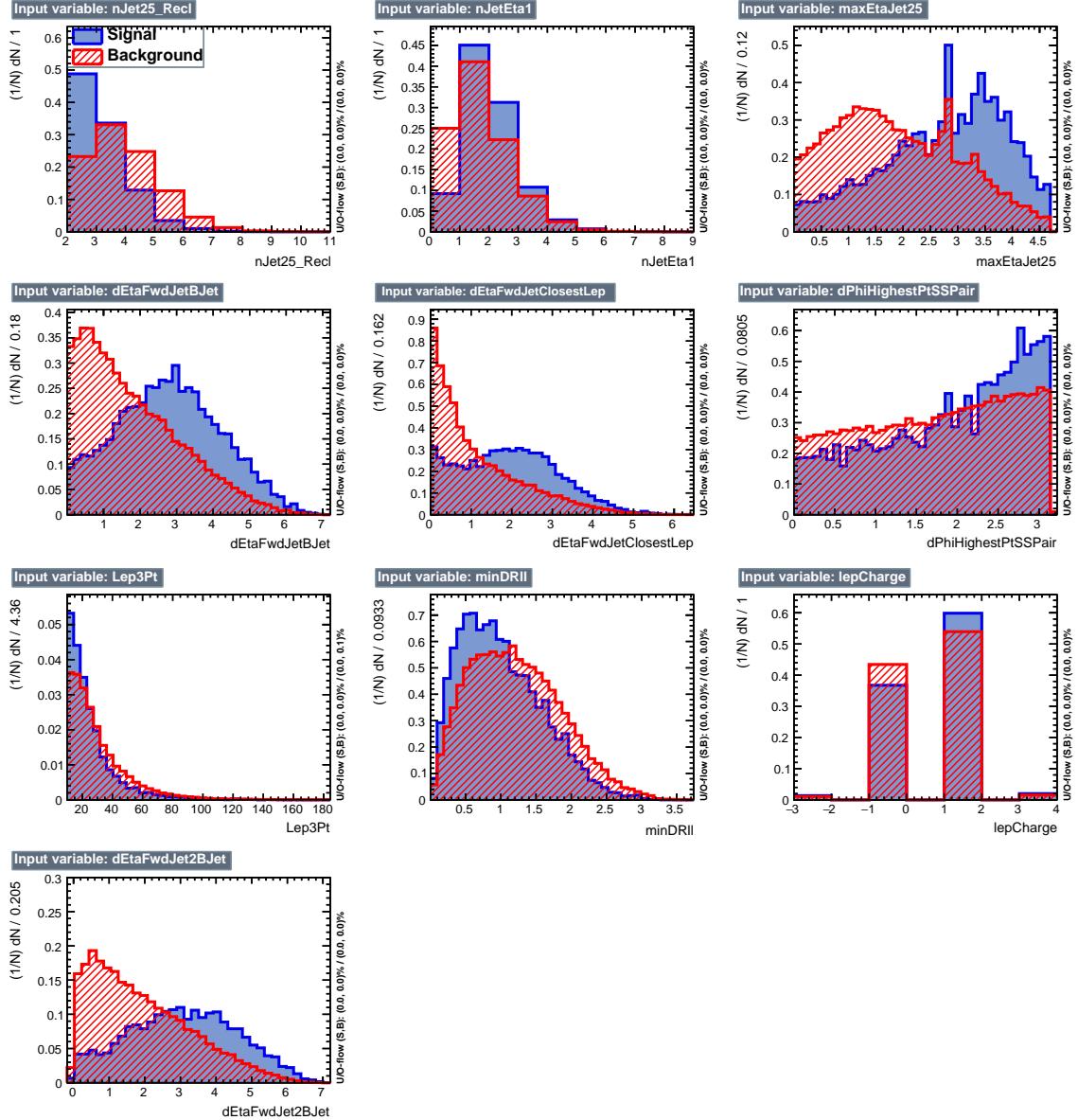
**Figure B.5:** BDT input variables as seen by BDTG classifier for the  $2lss$  channel,  $tHq$  signal (blue) discriminated against  $t\bar{t}$  background (red).



**Figure B.6:** BDT input variables as seen by BDTG classifier for the  $2lss$  channel,  $tHq$  signal(blue) discriminated against  $t\bar{t}V$  background (red).

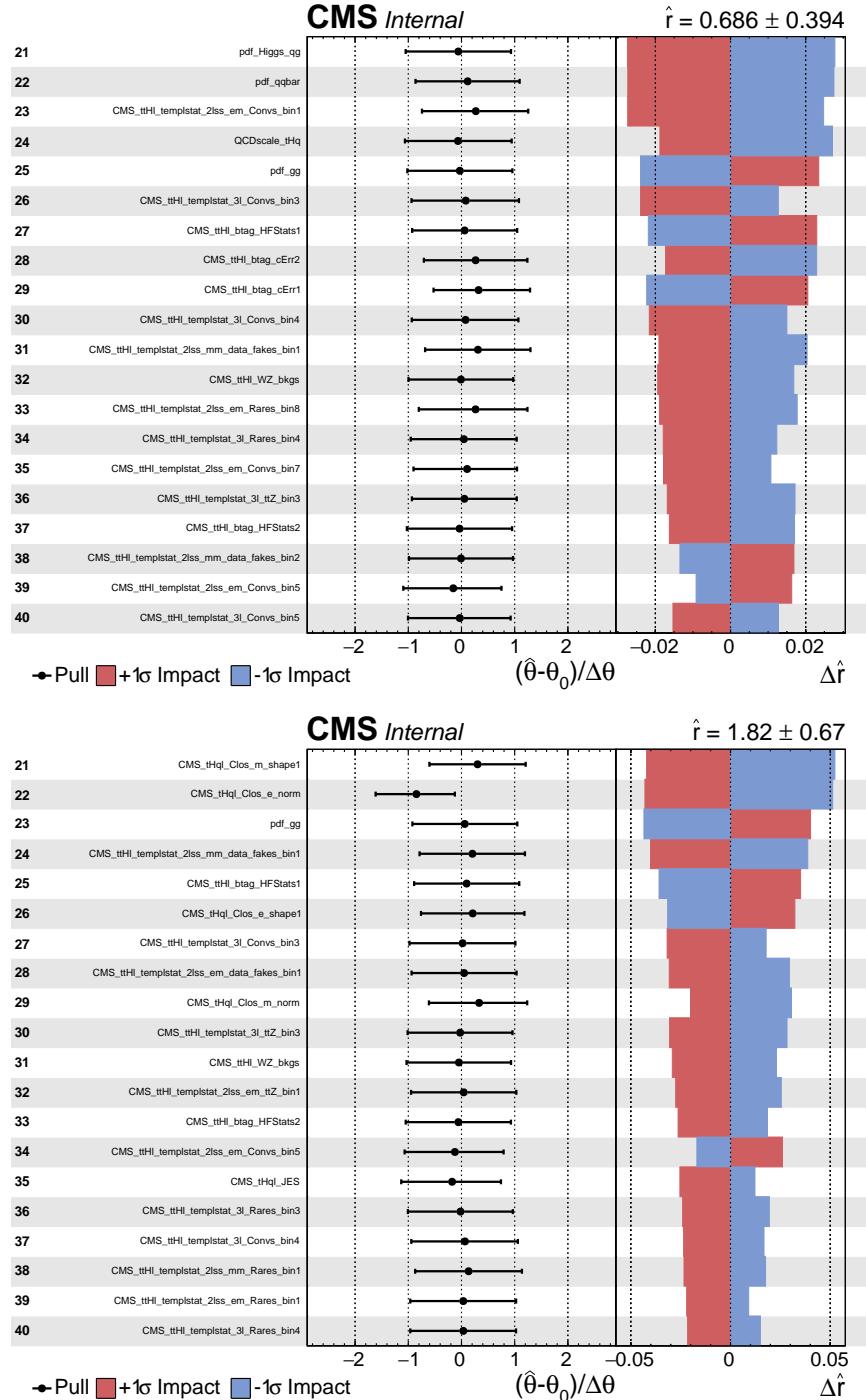


**Figure B.7:** BDT input variables as seen by BDTG classifier for the  $3l$  channel,  $tHq$  signal (blue) discriminated against  $t\bar{t}$  background (red).

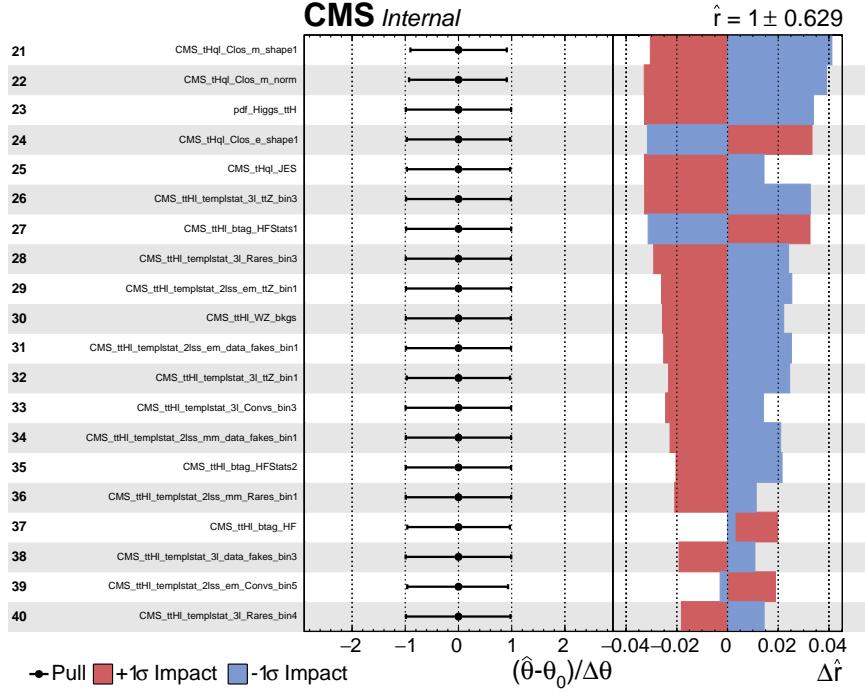


**Figure B.8:** BDT input variables as seen by BDTG classifier for the  $3l$  channel,  $tHq$  signal (blue) discriminated against  $t\bar{t}V$  background (red).

3606 B.4 Pulls and impacts



**Figure B.9:** Post-fit pulls and impacts of the next 20 nuisance parameters with largest impacts for the fit on the observed data, for the ITC (top) and SM (bottom) hypotheses.



**Figure B.10:** Post-fit pulls and impacts of the next 20 nuisance parameters with largest impacts for a fit to the Asimov dataset with fixed signal strength, for the  $\kappa_t/\kappa_V = -1.0$  hypothesis.

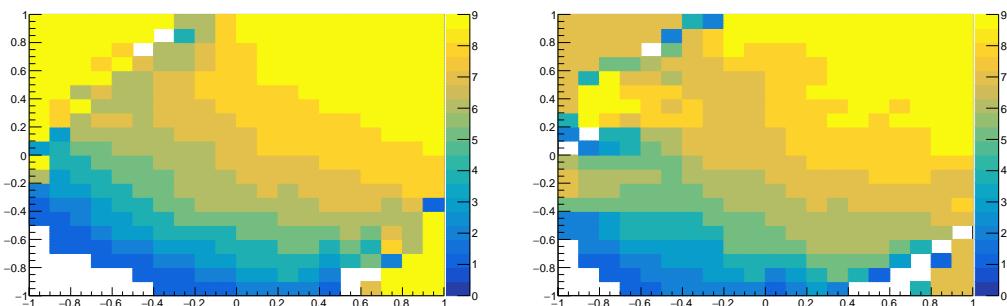
3607 **Appendix C**

3608 **Other binning strategies**

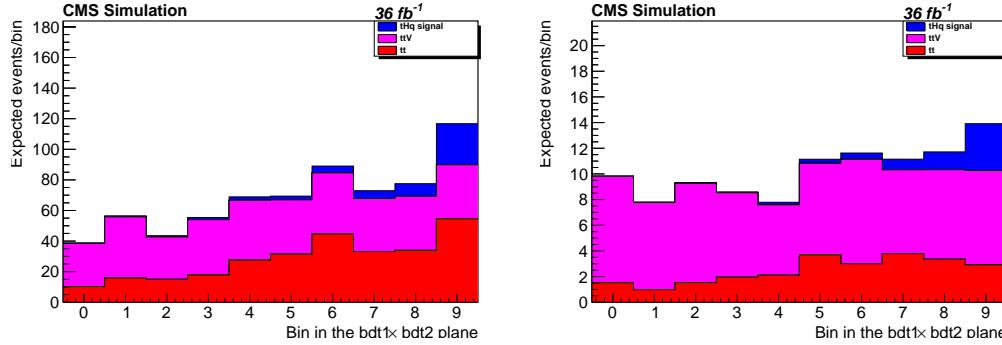
3609 Two additional strategies of clustering regions in the 2D plane of  $BDTG_{tt}$  vs  $BDTG_{ttV}$   
3610 into bins were attempted, following studies done and documented in great detail in  
3611 Reference [149]. A brief description is provided in the following.

3612 **Clustering by S/B ratio**

3613 In this method, the 2D plane is clustered into a given number of bins corresponding  
3614 to regions where S/B is within a certain range. The bin borders are determined  
3615 such that the number of background events in each bin is approximately equal. The  
3616 resulting regions for  $2lss$  and  $3l$  events are shown in Figure C.1, while the expected  
3617 distribution of signal and dominant backgrounds are shown in Figure C.2.



**Figure C.1:** Binning by S/B regions for  $2lss$  (left) and  $3l$  (right).



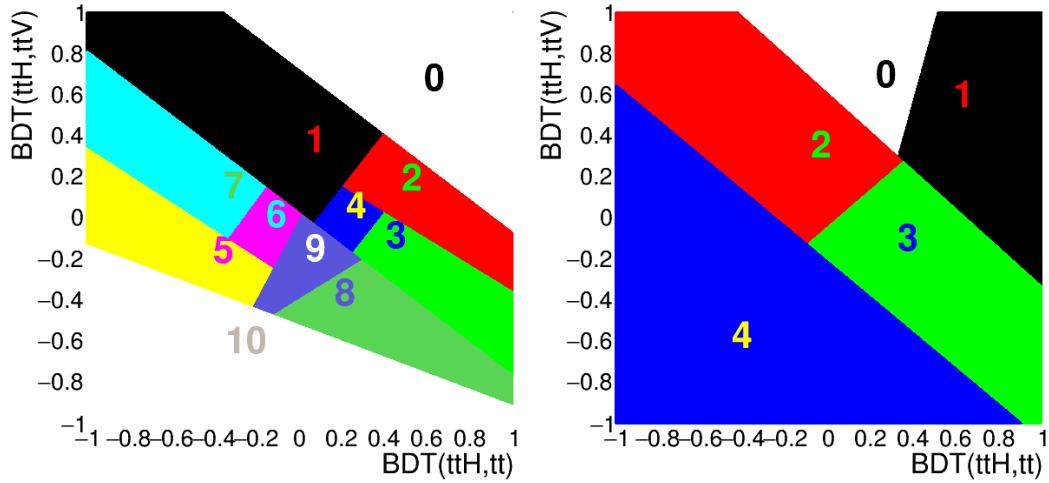
**Figure C.2:** Final bins (corresponding to S/B regions in the 2D plane) for  $2lss$  and  $3l$  (right).

Using this method, the resulting limits (for the  $\kappa_t = -1, \kappa_V = 1$  scenario) are about 20% worse than with the binning in Section 6.9.6:  $\mu^\pm\mu^\pm$  changed from 1.82 to 2.15,  $3l$  changed from 1.52 to 1.75.

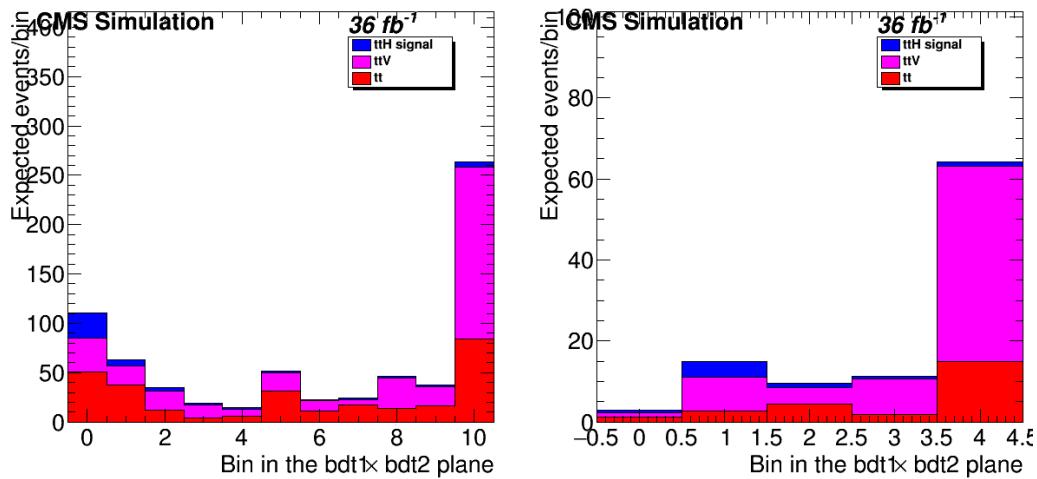
### ***k*-Means geometric clustering**

This method employs a recursive application of the *k*-means algorithm (see Appendix D in Reference [149]) to separate the 2D plane into geometric regions. The resulting clustering (using the  $t\bar{t}H$  multilepton code on  $tHq$  signal and  $t\bar{t}$  and  $t\bar{t}V$  background events) are shown in Figure C.3. The expected distribution of events for the signal and dominant backgrounds in these bins is shown in Fig. C.4.

Similarly to the S/B ratio binning, the limits using the *k*-means clustering are significantly worse than those of the bins described before. In the  $\mu^\pm\mu^\pm$  channel, the limit deteriorates from 1.82 to 2.05, whereas in  $3l$  it changes from 1.58 to 1.78.



**Figure C.3:** Binning into geometric regions using a  $k$ -means algorithm for  $2lss$  (left) and  $3l$  (right).

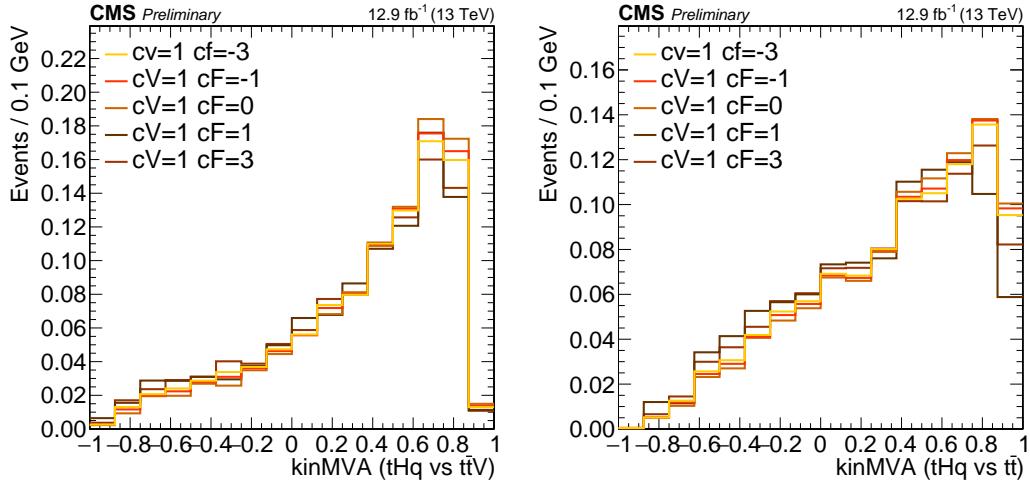


**Figure C.4:** Final bins using a  $k$ -means algorithm for  $2lss$  (left) and  $3l$  (right). Note that the bin numbering here is such that signal-like bins are lower.

3630 **Appendix D**

3631 **BDTG output variation with  $\kappa_V/\kappa_t$**

3632 The BDTG classifier output was described in Section in the  $\kappa_t = -1, \kappa_V = 1$  scenario; the  
 3633 change of BDTG classifiers output shape when varying the  $\kappa_V/\kappa_t$  coupling scenario  
 3634 is shown in Figure D.1 in the  $3l$  channel for five different values of  $\kappa_t$ , with  $\kappa_V$  fixed  
 at 1.0.



**Figure D.1:** Change of the BDTG classifiers output when varying  $\kappa_t$  coupling ( $\kappa_V$  is fixed at 1.0). Training vs.  $t\bar{t}V$  (right) and vs.  $t\bar{t}$  (left).

3635

3636 Given that the BDT classifier output shape does not change, it is enough to train  
 3637 the BDTG in one of the  $\kappa_t/\kappa_V$  points. It was chosen the SM point.

<sup>3638</sup> **Appendix E**

<sup>3639</sup>  **$tHq$ - $t\bar{t}H$  overlap**

<sup>3640</sup> This section provides a quick overview of the differences and commonalities in event  
<sup>3641</sup> selections between this analysis and the  $t\bar{t}H$  multilepton search [149]. The object  
<sup>3642</sup> selections of the two analysis are perfectly synchronized due to shared frameworks  
<sup>3643</sup> and samples. The only exception is the usage of forward jets ( $|\eta| > 2.4, p_T > 40$  GeV)  
<sup>3644</sup> in this analysis. Such jets are not considered in the  $t\bar{t}H$  analysis.

<sup>3645</sup> Table E.1 gives an overview of the main differences in the event selections. Here,  
<sup>3646</sup>  $E_T^{miss}_{LD}$  is defined as  $E_T^{miss} \times 0.00397 + H_T^{miss} \times 0.00265$ . Untagged jets in the  $tHq$   
<sup>3647</sup> analysis are jets that do not pass the CSV loose working point and are either central  
<sup>3648</sup> ( $|\eta| < 2.4, p_T > 25$  GeV) or forward ( $|\eta| < 2.4, p_T > 40$  GeV). All jets in the  $t\bar{t}H$  analysis  
<sup>3649</sup> are selected with  $p_T > 25$  GeV. Lepton  $p_T$  cuts and the trigger selections are identical.

Channel	$tHq$	$t\bar{t}H$
3l	Z veto, 15bGeV $N_{jets}^{\text{b, med.}} \geq 1$ $\geq 1$ un-tagged jet	Z veto, 10 GeV $N_{jets}^{\text{b, med.}} \geq 1$ OR $N_{jets}^{\text{b, loose}} \geq 2$ $E_T^{miss}_{LD} > 0.2$ OR $N_{\text{centrl.}} \geq 4$
2lss	$N_{jets}^{\text{b, med.}} \geq 1$ $\geq 1$ un-tagged jet	$N_{jets}^{\text{b, med.}} \geq 1$ OR $N_{jets}^{\text{b, loose}} \geq 2$ $N_{\text{central}} \geq 4$

**Table E.1:** Differences in event selection between this analysis and the  $t\bar{t}H$  multilepton analysis.

3650       Table E.2 shows the total events yields in the individual channels, and the yield  
 3651       of shared events between each channel, for the  $tHq$  signal sample, the  $t\bar{t}H$  signal  
 3652       sample, and the data. In the data, for the  $3l$  channel, about 80% of events passing  
 3653       the  $tHq$  selection also pass the  $t\bar{t}H$  selection, constituting about 70% of that channel.  
 3654       In the  $2lss$  channel, about 50% of data events passing the  $tHq$  selection also pass the  
 3655        $t\bar{t}H$  selection, but these events constitute almost 90% of the  $t\bar{t}H$  selection in those  
 3656       channels. Similar overlaps are also seen in the  $tHq$  and  $t\bar{t}H$  signal samples.

3657       There is no migration between different channels and different selections, i.e., no  
 3658       events passing the selection of a given  $tHq$  channel pass the selection of any other  
 3659       channels of  $t\bar{t}H$  and vice versa.

$tHq$ sample	$tHq$	$t\bar{t}H$	Common	(% $tHq$ )	(% $t\bar{t}H$ )
$\mu^\pm\mu^\pm$	7400	2353	2166	29.3	92.1
$e^\pm\mu^\pm$	11158	3600	3321	29.8	92.2
$e^\pm e^\pm$	3550	1106	1025	28.9	92.7
$\ell\ell\ell$	3115	2923	2347	75.3	80.3

$t\bar{t}H$ sample	$tHq$	$t\bar{t}H$	Common	(% $tHq$ )	(% $t\bar{t}H$ )
$\mu^\pm\mu^\pm$	32612	28703	26547	81.4	92.5
$e^\pm\mu^\pm$	48088	42521	39164	81.4	92.1
$e^\pm e^\pm$	15476	12869	11896	76.9	92.4
$\ell\ell\ell$	26627	30598	25288	95.0	82.6

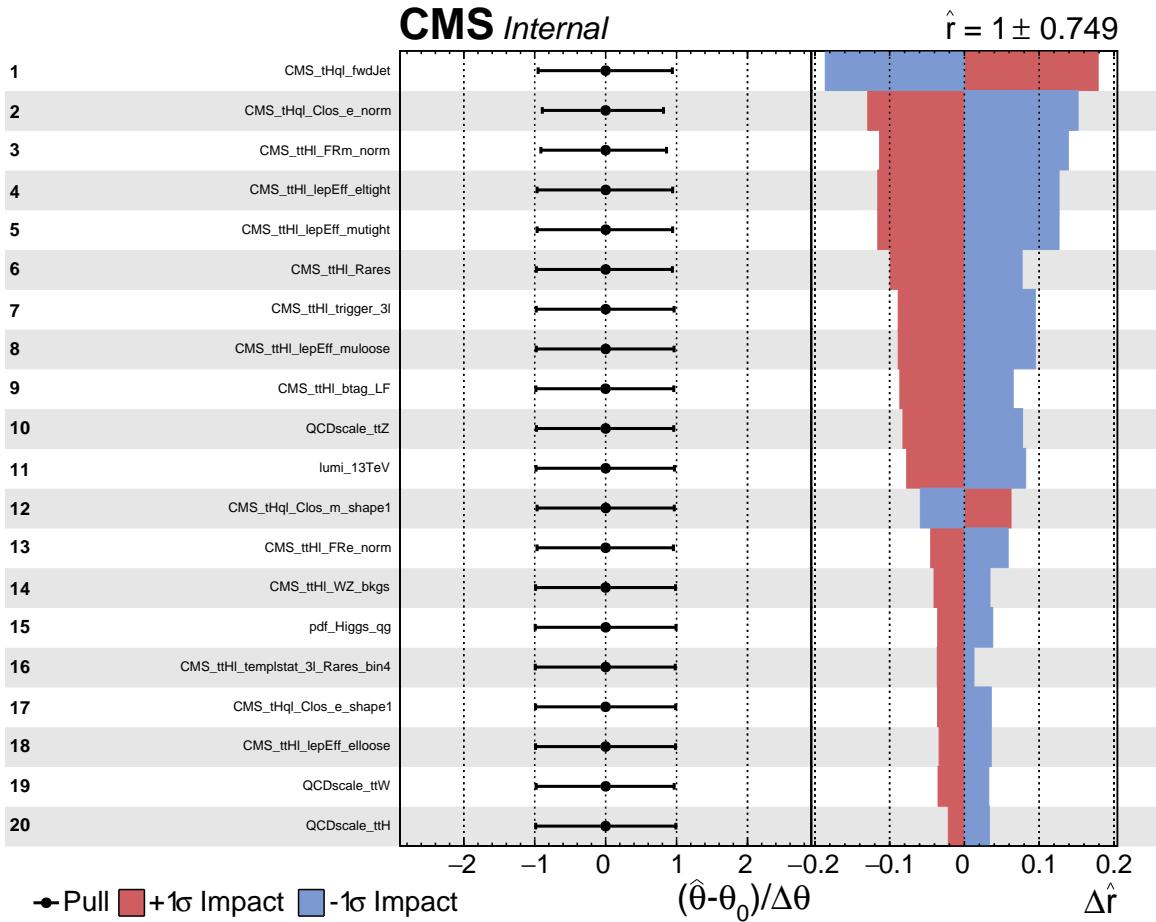
Data	$tHq$	$t\bar{t}H$	Common	(% $tHq$ )	(% $t\bar{t}H$ )
$\mu^\pm\mu^\pm$	280	160	140	50.0	87.5
$e^\pm\mu^\pm$	525	280	242	46.1	86.4
$e^\pm e^\pm$	208	90	79	38.0	87.8
$\ell\ell\ell$	126	154	104	82.5	67.5

**Table E.2:** Individual and shared event yields between this analysis ( $tHq$ ) and  $t\bar{t}H$  multilepton selections.

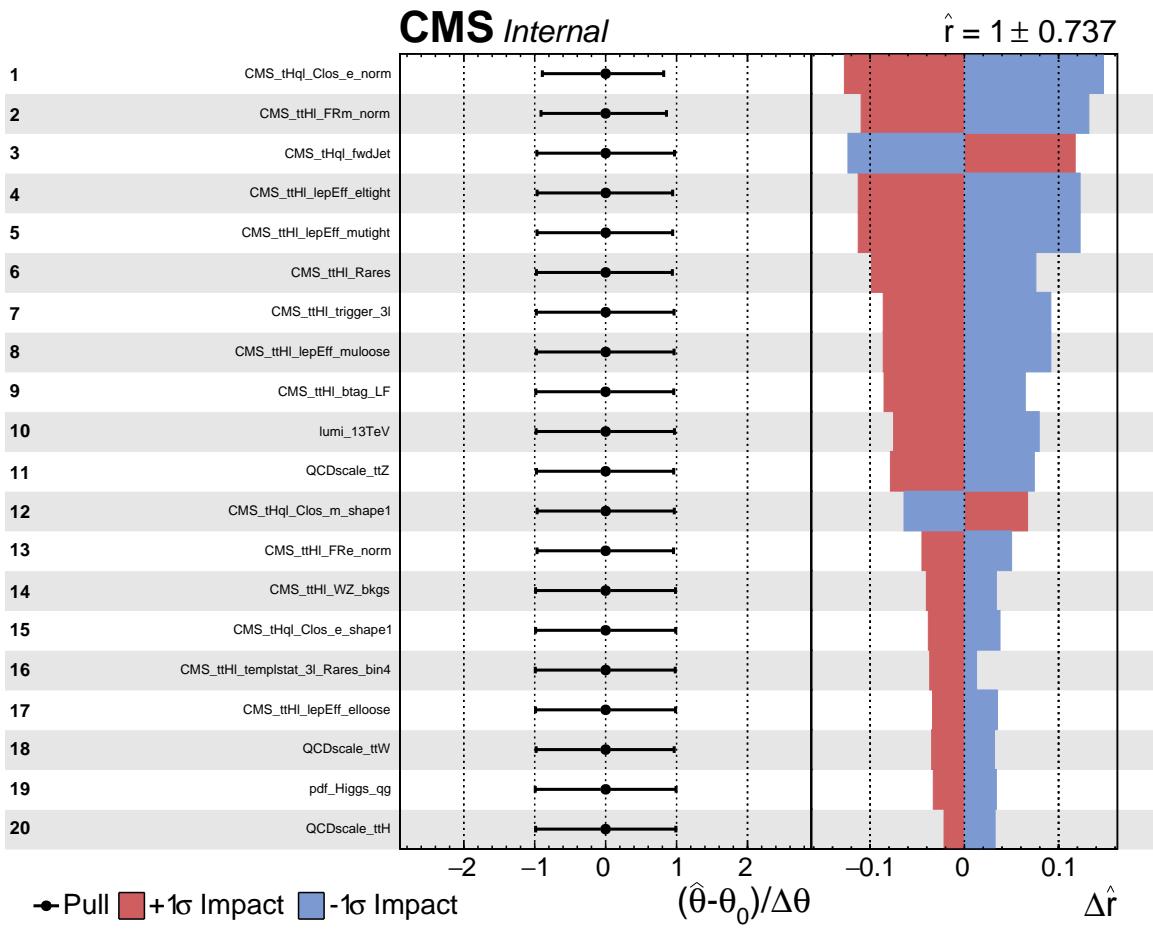
3660 **Appendix F**

3661 **Forward jet impact plots**

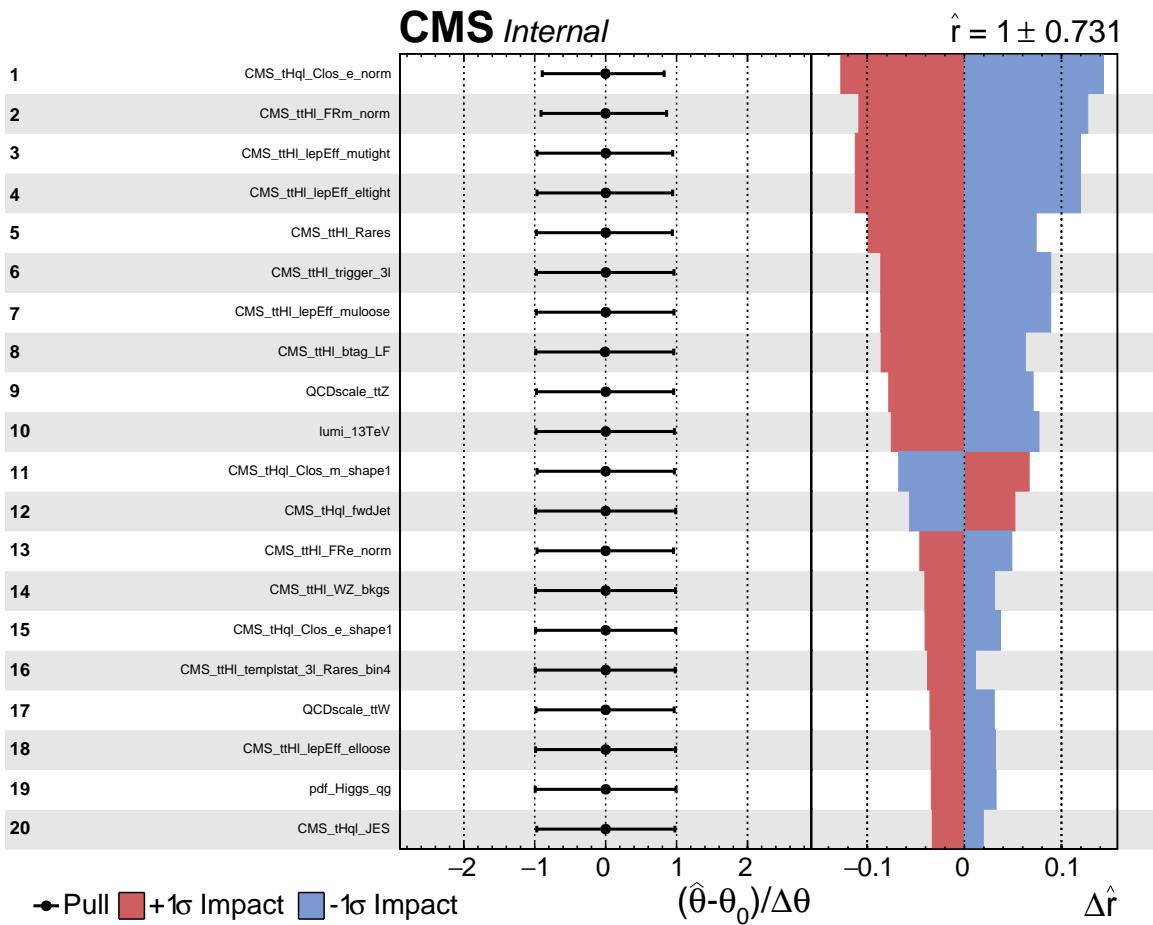
3662 The impact of the data/MC disagreement for forward jet  $\eta$  is observed to reduce with  
3663 higher  $p_T$  cuts; Figures F.1, F.2 and F.3 show this reduction in the impact of the  
3664 forward jet  $\eta$  nuisance in the fit.



**Figure F.1:** Post-fit pulls and impacts of the 20 nuisance parameters with  $p_T$  cut 25 GeV for the forward jet.



**Figure F.2:** Post-fit pulls and impacts of the 20 nuisance parameters with  $p_T$  cut 30 GeV for the forward jet.



**Figure F.3:** Post-fit pulls and impacts of the 20 nuisance parameters with  $p_T$  cut 40 GeV for the forward jet.

<sup>3665</sup> **Appendix G**

<sup>3666</sup> **Cross sections and Branching**

<sup>3667</sup> **ratios scalings**

$\kappa_V$	$\kappa_t$	HWW	HZZ	H $\tau\tau$	H $\mu\mu$	Hbb	Hcc	H $\gamma\gamma$	HZ $\gamma$	Hgg
0.5	-6.0	0.0827	0.0827	11.9098	11.9098	0.3308	0.3308	0.3308	0.3308	0.3308
0.5	-4.0	0.1417	0.1417	9.0699	9.0699	0.5669	0.5669	0.5669	0.5669	0.5669
0.5	-3.0	0.1889	0.1889	6.7999	6.7999	0.7555	0.7555	0.7555	0.7555	0.7555
0.5	-2.5	0.2173	0.2173	5.4325	5.4325	0.8692	0.8692	0.8692	0.8692	0.8692
0.5	-2.0	0.2478	0.2478	3.9647	3.9647	0.9912	0.9912	0.9912	0.9912	0.9912
0.5	-1.5	0.2782	0.2782	2.5034	2.5034	1.1126	1.1126	1.1126	1.1126	1.1126
0.5	-1.333	0.2877	0.2877	2.0448	2.0448	1.1508	1.1508	1.1508	1.1508	1.1508
0.5	-1.25	0.2922	0.2922	1.8264	1.8264	1.1689	1.1689	1.1689	1.1689	1.1689
0.5	-1.0	0.3048	0.3048	1.2194	1.2194	1.2194	1.2194	1.2194	1.2194	1.2194
0.5	-0.833	0.3122	0.3122	0.8665	0.8665	1.2487	1.2487	1.2487	1.2487	1.2487
0.5	-0.75	0.3154	0.3154	0.7097	0.7097	1.2617	1.2617	1.2617	1.2617	1.2617
0.5	-0.667	0.3184	0.3184	0.5666	0.5666	1.2736	1.2736	1.2736	1.2736	1.2736
0.5	-0.5	0.3235	0.3235	0.3235	0.3235	1.2938	1.2938	1.2938	1.2938	1.2938
0.5	-0.333	0.3272	0.3272	0.1451	0.1451	1.3087	1.3087	1.3087	1.3087	1.3087
0.5	-0.25	0.3285	0.3285	0.0821	0.0821	1.3139	1.3139	1.3139	1.3139	1.3139
0.5	-0.167	0.3294	0.3294	0.0367	0.0367	1.3177	1.3177	1.3177	1.3177	1.3177
0.5	0.0	0.3302	0.3302	0.0000	0.0000	1.3207	1.3207	1.3207	1.3207	1.3207
0.5	0.167	0.3294	0.3294	0.0367	0.0367	1.3177	1.3177	1.3177	1.3177	1.3177
0.5	0.25	0.3285	0.3285	0.0821	0.0821	1.3139	1.3139	1.3139	1.3139	1.3139
0.5	0.333	0.3272	0.3272	0.1451	0.1451	1.3087	1.3087	1.3087	1.3087	1.3087
0.5	0.5	0.3235	0.3235	0.3235	0.3235	1.2938	1.2938	1.2938	1.2938	1.2938
0.5	0.667	0.3184	0.3184	0.5666	0.5666	1.2736	1.2736	1.2736	1.2736	1.2736
0.5	0.75	0.3154	0.3154	0.7097	0.7097	1.2617	1.2617	1.2617	1.2617	1.2617
0.5	0.833	0.3122	0.3122	0.8665	0.8665	1.2487	1.2487	1.2487	1.2487	1.2487
0.5	1.0	0.3048	0.3048	1.2194	1.2194	1.2194	1.2194	1.2194	1.2194	1.2194
0.5	1.25	0.2922	0.2922	1.8264	1.8264	1.1689	1.1689	1.1689	1.1689	1.1689
0.5	1.333	0.2877	0.2877	2.0448	2.0448	1.1508	1.1508	1.1508	1.1508	1.1508
0.5	1.5	0.2782	0.2782	2.5034	2.5034	1.1126	1.1126	1.1126	1.1126	1.1126
0.5	2.0	0.2478	0.2478	3.9647	3.9647	0.9912	0.9912	0.9912	0.9912	0.9912
0.5	2.5	0.2173	0.2173	5.4325	5.4325	0.8692	0.8692	0.8692	0.8692	0.8692
0.5	3.0	0.1889	0.1889	6.7999	6.7999	0.7555	0.7555	0.7555	0.7555	0.7555
0.5	4.0	0.1417	0.1417	9.0699	9.0699	0.5669	0.5669	0.5669	0.5669	0.5669
0.5	6.0	0.0827	0.0827	11.9098	11.9098	0.3308	0.3308	0.3308	0.3308	0.3308

**Table G.1:** Scalings of Higgs decay branching ratios vs.  $\kappa_t$  and  $\kappa_V = 0.5$  for the non-resolved model.

$\kappa_V$	$\kappa_t$	HWW	HZZ	H $\tau\tau$	H $\mu\mu$	Hbb	Hcc	H $\gamma\gamma$	HZ $\gamma$	Hgg
1.0	-6.0	0.3122	0.3122	11.2408	11.2408	0.3122	0.3122	0.3122	0.3122	0.3122
1.0	-4.0	0.5144	0.5144	8.2305	8.2305	0.5144	0.5144	0.5144	0.5144	0.5144
1.0	-3.0	0.6651	0.6651	5.9862	5.9862	0.6651	0.6651	0.6651	0.6651	0.6651
1.0	-2.5	0.7517	0.7517	4.6979	4.6979	0.7517	0.7517	0.7517	0.7517	0.7517
1.0	-2.0	0.8412	0.8412	3.3647	3.3647	0.8412	0.8412	0.8412	0.8412	0.8412
1.0	-1.5	0.9271	0.9271	2.0859	2.0859	0.9271	0.9271	0.9271	0.9271	0.9271
1.0	-1.333	0.9534	0.9534	1.6941	1.6941	0.9534	0.9534	0.9534	0.9534	0.9534
1.0	-1.25	0.9658	0.9658	1.5091	1.5091	0.9658	0.9658	0.9658	0.9658	0.9658
1.0	-1.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1.0	-0.833	1.0196	1.0196	0.7075	0.7075	1.0196	1.0196	1.0196	1.0196	1.0196
1.0	-0.75	1.0283	1.0283	0.5784	0.5784	1.0283	1.0283	1.0283	1.0283	1.0283
1.0	-0.667	1.0362	1.0362	0.4610	0.4610	1.0362	1.0362	1.0362	1.0362	1.0362
1.0	-0.5	1.0495	1.0495	0.2624	0.2624	1.0495	1.0495	1.0495	1.0495	1.0495
1.0	-0.333	1.0593	1.0593	0.1175	0.1175	1.0593	1.0593	1.0593	1.0593	1.0593
1.0	-0.25	1.0627	1.0627	0.0664	0.0664	1.0627	1.0627	1.0627	1.0627	1.0627
1.0	-0.167	1.0652	1.0652	0.0297	0.0297	1.0652	1.0652	1.0652	1.0652	1.0652
1.0	0.0	1.0672	1.0672	0.0000	0.0000	1.0672	1.0672	1.0672	1.0672	1.0672
1.0	0.167	1.0652	1.0652	0.0297	0.0297	1.0652	1.0652	1.0652	1.0652	1.0652
1.0	0.25	1.0627	1.0627	0.0664	0.0664	1.0627	1.0627	1.0627	1.0627	1.0627
1.0	0.333	1.0593	1.0593	0.1175	0.1175	1.0593	1.0593	1.0593	1.0593	1.0593
1.0	0.5	1.0495	1.0495	0.2624	0.2624	1.0495	1.0495	1.0495	1.0495	1.0495
1.0	0.667	1.0362	1.0362	0.4610	0.4610	1.0362	1.0362	1.0362	1.0362	1.0362
1.0	0.75	1.0283	1.0283	0.5784	0.5784	1.0283	1.0283	1.0283	1.0283	1.0283
1.0	0.833	1.0196	1.0196	0.7075	0.7075	1.0196	1.0196	1.0196	1.0196	1.0196
1.0	1.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1.0	1.25	0.9658	0.9658	1.5091	1.5091	0.9658	0.9658	0.9658	0.9658	0.9658
1.0	1.333	0.9534	0.9534	1.6941	1.6941	0.9534	0.9534	0.9534	0.9534	0.9534
1.0	1.5	0.9271	0.9271	2.0859	2.0859	0.9271	0.9271	0.9271	0.9271	0.9271
1.0	2.0	0.8412	0.8412	3.3647	3.3647	0.8412	0.8412	0.8412	0.8412	0.8412
1.0	2.5	0.7517	0.7517	4.6979	4.6979	0.7517	0.7517	0.7517	0.7517	0.7517
1.0	3.0	0.6651	0.6651	5.9862	5.9862	0.6651	0.6651	0.6651	0.6651	0.6651
1.0	4.0	0.5144	0.5144	8.2305	8.2305	0.5144	0.5144	0.5144	0.5144	0.5144
1.0	6.0	0.3122	0.3122	11.2408	11.2408	0.3122	0.3122	0.3122	0.3122	0.3122

**Table G.2:** Scalings of Higgs decay branching ratios vs.  $\kappa_t$  and  $\kappa_V = 1.0$  for the non-resolved model.

$\kappa_V$	$\kappa_t$	HWW	HZZ	H $\tau\tau$	H $\mu\mu$	Hbb	Hcc	H $\gamma\gamma$	HZ $\gamma$	Hgg
1.5	-6.0	0.6424	0.6424	10.2785	10.2785	0.2855	0.2855	0.2855	0.2855	0.2855
1.5	-4.0	1.0028	1.0028	7.1307	7.1307	0.4457	0.4457	0.4457	0.4457	0.4457
1.5	-3.0	1.2477	1.2477	4.9909	4.9909	0.5545	0.5545	0.5545	0.5545	0.5545
1.5	-2.5	1.3802	1.3802	3.8338	3.8338	0.6134	0.6134	0.6134	0.6134	0.6134
1.5	-2.0	1.5115	1.5115	2.6870	2.6870	0.6718	0.6718	0.6718	0.6718	0.6718
1.5	-1.5	1.6322	1.6322	1.6322	1.6322	0.7254	0.7254	0.7254	0.7254	0.7254
1.5	-1.333	1.6682	1.6682	1.3175	1.3175	0.7414	0.7414	0.7414	0.7414	0.7414
1.5	-1.25	1.6851	1.6851	1.1702	1.1702	0.7489	0.7489	0.7489	0.7489	0.7489
1.5	-1.0	1.7310	1.7310	0.7693	0.7693	0.7693	0.7693	0.7693	0.7693	0.7693
1.5	-0.833	1.7570	1.7570	0.5419	0.5419	0.7809	0.7809	0.7809	0.7809	0.7809
1.5	-0.75	1.7684	1.7684	0.4421	0.4421	0.7860	0.7860	0.7860	0.7860	0.7860
1.5	-0.667	1.7788	1.7788	0.3517	0.3517	0.7906	0.7906	0.7906	0.7906	0.7906
1.5	-0.5	1.7962	1.7962	0.1996	0.1996	0.7983	0.7983	0.7983	0.7983	0.7983
1.5	-0.333	1.8089	1.8089	0.0891	0.0891	0.8039	0.8039	0.8039	0.8039	0.8039
1.5	-0.25	1.8133	1.8133	0.0504	0.0504	0.8059	0.8059	0.8059	0.8059	0.8059
1.5	-0.167	1.8165	1.8165	0.0225	0.0225	0.8073	0.8073	0.8073	0.8073	0.8073
1.5	0.0	1.8191	1.8191	0.0000	0.0000	0.8085	0.8085	0.8085	0.8085	0.8085
1.5	0.167	1.8165	1.8165	0.0225	0.0225	0.8073	0.8073	0.8073	0.8073	0.8073
1.5	0.25	1.8133	1.8133	0.0504	0.0504	0.8059	0.8059	0.8059	0.8059	0.8059
1.5	0.333	1.8089	1.8089	0.0891	0.0891	0.8039	0.8039	0.8039	0.8039	0.8039
1.5	0.5	1.7962	1.7962	0.1996	0.1996	0.7983	0.7983	0.7983	0.7983	0.7983
1.5	0.667	1.7788	1.7788	0.3517	0.3517	0.7906	0.7906	0.7906	0.7906	0.7906
1.5	0.75	1.7684	1.7684	0.4421	0.4421	0.7860	0.7860	0.7860	0.7860	0.7860
1.5	0.833	1.7570	1.7570	0.5419	0.5419	0.7809	0.7809	0.7809	0.7809	0.7809
1.5	1.0	1.7310	1.7310	0.7693	0.7693	0.7693	0.7693	0.7693	0.7693	0.7693
1.5	1.25	1.6851	1.6851	1.1702	1.1702	0.7489	0.7489	0.7489	0.7489	0.7489
1.5	1.333	1.6682	1.6682	1.3175	1.3175	0.7414	0.7414	0.7414	0.7414	0.7414
1.5	1.5	1.6322	1.6322	1.6322	1.6322	0.7254	0.7254	0.7254	0.7254	0.7254
1.5	2.0	1.5115	1.5115	2.6870	2.6870	0.6718	0.6718	0.6718	0.6718	0.6718
1.5	2.5	1.3802	1.3802	3.8338	3.8338	0.6134	0.6134	0.6134	0.6134	0.6134
1.5	3.0	1.2477	1.2477	4.9909	4.9909	0.5545	0.5545	0.5545	0.5545	0.5545
1.5	4.0	1.0028	1.0028	7.1307	7.1307	0.4457	0.4457	0.4457	0.4457	0.4457
1.5	6.0	0.6424	0.6424	10.2785	10.2785	0.2855	0.2855	0.2855	0.2855	0.2855

**Table G.3:** Scalings of Higgs decay branching ratios vs.  $\kappa_t$  and  $\kappa_V = 1.5$  for the non-resolved model.

$\kappa_V$	$\kappa_t$	ttHWW	ttHZZ	ttH $\tau\tau$	tHqWW	tHqZZ	tHq $\tau\tau$	tHWWW	tHWZZ	tHW $\tau\tau$
0.5	-6.0	2.9775	2.9775	428.7530	9.2066	9.2066	1325.7460	9.7660	9.7660	1406.3049
0.5	-4.0	2.2675	2.2675	145.1182	7.5740	7.5740	484.7357	7.8819	7.8819	504.4411
0.5	-3.0	1.7000	1.7000	61.1988	6.1214	6.1214	220.3702	6.2562	6.2562	225.2227
0.5	-2.5	1.3581	1.3581	33.9529	5.1857	5.1857	129.6430	5.2277	5.2277	130.6931
0.5	-2.0	0.9912	0.9912	15.8589	4.1227	4.1227	65.9633	4.0762	4.0762	65.2197
0.5	-1.5	0.6259	0.6259	5.6327	2.9838	2.9838	26.8544	2.8645	2.8645	25.7805
0.5	-1.333	0.5112	0.5112	3.6333	2.6025	2.6025	18.4974	2.4648	2.4648	17.5190
0.5	-1.25	0.4566	0.4566	2.8538	2.4154	2.4154	15.0962	2.2700	2.2700	14.1878
0.5	-1.0	0.3048	0.3048	1.2194	1.8696	1.8696	7.4784	1.7078	1.7078	6.8310
0.5	-0.833	0.2166	0.2166	0.6012	1.5271	1.5271	4.2386	1.3605	1.3605	3.7760
0.5	-0.75	0.1774	0.1774	0.3992	1.3657	1.3657	3.0729	1.1987	1.1987	2.6970
0.5	-0.667	0.1417	0.1417	0.2521	1.2111	1.2111	2.1553	1.0451	1.0451	1.8598
0.5	-0.5	0.0809	0.0809	0.0809	0.9236	0.9236	0.9236	0.7640	0.7640	0.7640
0.5	-0.333	0.0363	0.0363	0.0161	0.6720	0.6720	0.2981	0.5249	0.5249	0.2328
0.5	-0.25	0.0205	0.0205	0.0051	0.5618	0.5618	0.1405	0.4231	0.4231	0.1058
0.5	-0.167	0.0092	0.0092	0.0010	0.4622	0.4622	0.0516	0.3334	0.3334	0.0372
0.5	0.0	0.0000	0.0000	0.0000	0.2953	0.2953	0.0000	0.1909	0.1909	0.0000
0.5	0.167	0.0092	0.0092	0.0010	0.1755	0.1755	0.0196	0.1010	0.1010	0.0113
0.5	0.25	0.0205	0.0205	0.0051	0.1339	0.1339	0.0335	0.0762	0.0762	0.0191
0.5	0.333	0.0363	0.0363	0.0161	0.1043	0.1043	0.0463	0.0647	0.0647	0.0287
0.5	0.5	0.0809	0.0809	0.0809	0.0809	0.0809	0.0809	0.0809	0.0809	0.0809
0.5	0.667	0.1417	0.1417	0.2521	0.1044	0.1044	0.1859	0.1480	0.1480	0.2634
0.5	0.75	0.1774	0.1774	0.3992	0.1329	0.1329	0.2991	0.1993	0.1993	0.4485
0.5	0.833	0.2166	0.2166	0.6012	0.1720	0.1720	0.4775	0.2620	0.2620	0.7272
0.5	1.0	0.3048	0.3048	1.2194	0.2811	0.2811	1.1243	0.4200	0.4200	1.6801
0.5	1.25	0.4566	0.4566	2.8538	0.5119	0.5119	3.1993	0.7270	0.7270	4.5438
0.5	1.333	0.5112	0.5112	3.6333	0.6041	0.6041	4.2939	0.8449	0.8449	6.0051
0.5	1.5	0.6259	0.6259	5.6327	0.8096	0.8096	7.2863	1.1020	1.1020	9.9179
0.5	2.0	0.9912	0.9912	15.8589	1.5402	1.5402	24.6428	1.9827	1.9827	31.7238
0.5	2.5	1.3581	1.3581	33.9529	2.3549	2.3549	58.8716	2.9329	2.9329	73.3233
0.5	3.0	1.7000	1.7000	61.1988	3.1686	3.1686	114.0678	3.8625	3.8625	139.0502
0.5	4.0	2.2675	2.2675	145.1182	4.6200	4.6200	295.6829	5.4873	5.4873	351.1881
0.5	6.0	2.9775	2.9775	428.7530	6.6207	6.6207	953.3740	7.6698	7.6698	1104.4467

**Table G.4:** Scalings of cross section times BR for the non-resolved model, for the different  $t\bar{t}H$ ,  $tHq$ ,  $tHW$  signal components and  $\kappa_V = 0.5$ .

$\kappa_V$	$\kappa_t$	ttHWW	ttHZZ	ttH $\tau\tau$	tHqWW	tHqZZ	tHq $\tau\tau$	tHWWW	tHWZZ	tHW $\tau\tau$
1.0	-6.0	11.2408	11.2408	404.6686	40.4768	40.4768	1457.1666	41.3681	41.3681	1489.2533
1.0	-4.0	8.2305	8.2305	131.6886	34.2339	34.2339	547.7422	33.8480	33.8480	541.5676
1.0	-3.0	5.9862	5.9862	53.8759	28.5396	28.5396	256.8562	27.3983	27.3983	246.5850
1.0	-2.5	4.6979	4.6979	29.3616	24.8511	24.8511	155.3195	23.3557	23.3557	145.9734
1.0	-2.0	3.3647	3.3647	13.4590	20.6360	20.6360	82.5440	18.8497	18.8497	75.3987
1.0	-1.5	2.0859	2.0859	4.6933	16.0557	16.0557	36.1254	14.0919	14.0919	31.7068
1.0	-1.333	1.6941	1.6941	3.0102	14.4942	14.4942	25.7545	12.5059	12.5059	22.2216
1.0	-1.25	1.5091	1.5091	2.3579	13.7201	13.7201	21.4377	11.7273	11.7273	18.3239
1.0	-1.0	1.0000	1.0000	1.0000	11.4220	11.4220	11.4220	9.4484	9.4484	9.4484
1.0	-0.833	0.7075	0.7075	0.4909	9.9372	9.9372	6.8953	8.0059	8.0059	5.5552
1.0	-0.75	0.5784	0.5784	0.3254	9.2212	9.2212	5.1869	7.3200	7.3200	4.1175
1.0	-0.667	0.4610	0.4610	0.2051	8.5229	8.5229	3.7917	6.6579	6.6579	2.9620
1.0	-0.5	0.2624	0.2624	0.0656	7.1807	7.1807	1.7952	5.4076	5.4076	1.3519
1.0	-0.333	0.1175	0.1175	0.0130	5.9375	5.9375	0.6584	4.2814	4.2814	0.4748
1.0	-0.25	0.0664	0.0664	0.0042	5.3616	5.3616	0.3351	3.7730	3.7730	0.2358
1.0	-0.167	0.0297	0.0297	0.0008	4.8163	4.8163	0.1343	3.3009	3.3009	0.0921
1.0	0.0	0.0000	0.0000	0.0000	3.8183	3.8183	0.0000	2.4676	2.4676	0.0000
1.0	0.167	0.0297	0.0297	0.0008	2.9624	2.9624	0.0826	1.7981	1.7981	0.0501
1.0	0.25	0.0664	0.0664	0.0042	2.5928	2.5928	0.1620	1.5284	1.5284	0.0955
1.0	0.333	0.1175	0.1175	0.0130	2.2612	2.2612	0.2507	1.3014	1.3014	0.1443
1.0	0.5	0.2624	0.2624	0.0656	1.7115	1.7115	0.4279	0.9742	0.9742	0.2435
1.0	0.667	0.4610	0.4610	0.2051	1.3198	1.3198	0.5871	0.8188	0.8188	0.3643
1.0	0.75	0.5784	0.5784	0.3254	1.1834	1.1834	0.6657	0.8042	0.8042	0.4524
1.0	0.833	0.7075	0.7075	0.4909	1.0852	1.0852	0.7530	0.8301	0.8301	0.5760
1.0	1.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1.0	1.25	1.5091	1.5091	2.3579	1.1380	1.1380	1.7782	1.5278	1.5278	2.3872
1.0	1.333	1.6941	1.6941	3.0102	1.2492	1.2492	2.2197	1.7691	1.7691	3.1434
1.0	1.5	2.0859	2.0859	4.6933	1.5628	1.5628	3.5163	2.3434	2.3434	5.2727
1.0	2.0	3.3647	3.3647	13.4590	3.1023	3.1023	12.4092	4.6362	4.6362	18.5449
1.0	2.5	4.6979	4.6979	29.3616	5.2667	5.2667	32.9167	7.4799	7.4799	46.7493
1.0	3.0	5.9862	5.9862	53.8759	7.7435	7.7435	69.6914	10.5403	10.5403	94.8625
1.0	4.0	8.2305	8.2305	131.6886	12.7892	12.7892	204.6276	16.4642	16.4642	263.4266
1.0	6.0	11.2408	11.2408	404.6686	20.9516	20.9516	754.2573	25.5403	25.5403	919.4497

**Table G.5:** Scalings of cross section times BR for the non-resolved model, for the different  $t\bar{t}H$ ,  $tHq$ ,  $tHW$  signal components and  $\kappa_V = 1.0$ .

$\kappa_V$	$\kappa_t$	ttHWW	ttHZZ	ttH $\tau\tau$	tHqWW	tHqZZ	tHq $\tau\tau$	tHWWW	tHWZZ	tHW $\tau\tau$
1.5	-6.0	23.1266	23.1266	370.0260	96.1923	96.1923	1539.0768	95.1080	95.1080	1521.7272
1.5	-4.0	16.0441	16.0441	114.0913	81.6690	81.6690	580.7570	77.3512	77.3512	550.0531
1.5	-3.0	11.2295	11.2295	44.9178	68.8703	68.8703	275.4812	62.9086	62.9086	251.6344
1.5	-2.5	8.6261	8.6261	23.9614	60.7939	60.7939	168.8720	54.1622	54.1622	150.4505
1.5	-2.0	6.0458	6.0458	10.7481	51.7152	51.7152	91.9381	44.6227	44.6227	79.3293
1.5	-1.5	3.6725	3.6725	3.6725	41.9469	41.9469	41.9469	34.6991	34.6991	34.6991
1.5	-1.333	2.9643	2.9643	2.3410	38.6171	38.6171	30.4971	31.4016	31.4016	24.7987
1.5	-1.25	2.6330	2.6330	1.8284	36.9629	36.9629	25.6687	29.7807	29.7807	20.6810
1.5	-1.0	1.7310	1.7310	0.7693	32.0233	32.0233	14.2326	25.0144	25.0144	11.1175
1.5	-0.833	1.2192	1.2192	0.3760	28.7953	28.7953	8.8803	21.9653	21.9653	6.7740
1.5	-0.75	0.9948	0.9948	0.2487	27.2234	27.2234	6.8058	20.5014	20.5014	5.1254
1.5	-0.667	0.7914	0.7914	0.1565	25.6778	25.6778	5.0772	19.0767	19.0767	3.7720
1.5	-0.5	0.4491	0.4491	0.0499	22.6628	22.6628	2.5181	16.3435	16.3435	1.8159
1.5	-0.333	0.2006	0.2006	0.0099	19.7986	19.7986	0.9758	13.8117	13.8117	0.6807
1.5	-0.25	0.1133	0.1133	0.0031	18.4397	18.4397	0.5122	12.6364	12.6364	0.3510
1.5	-0.167	0.0507	0.0507	0.0006	17.1281	17.1281	0.2123	11.5203	11.5203	0.1428
1.5	0.0	0.0000	0.0000	0.0000	14.6443	14.6443	0.0000	9.4640	9.4640	0.0000
1.5	0.167	0.0507	0.0507	0.0006	12.3858	12.3858	0.1535	7.6760	7.6760	0.0951
1.5	0.25	0.1133	0.1133	0.0031	11.3529	11.3529	0.3154	6.8916	6.8916	0.1914
1.5	0.333	0.2006	0.2006	0.0099	10.3820	10.3820	0.5117	6.1783	6.1783	0.3045
1.5	0.5	0.4491	0.4491	0.0499	8.6227	8.6227	0.9581	4.9621	4.9621	0.5513
1.5	0.667	0.7914	0.7914	0.1565	7.1299	7.1299	1.4098	4.0411	4.0411	0.7990
1.5	0.75	0.9948	0.9948	0.2487	6.4888	6.4888	1.6222	3.6932	3.6932	0.9233
1.5	0.833	1.2192	1.2192	0.3760	5.9148	5.9148	1.8241	3.4176	3.4176	1.0540
1.5	1.0	1.7310	1.7310	0.7693	4.9627	4.9627	2.2057	3.0782	3.0782	1.3681
1.5	1.25	2.6330	2.6330	1.8284	4.0340	4.0340	2.8014	3.0873	3.0873	2.1440
1.5	1.333	2.9643	2.9643	2.3410	3.8531	3.8531	3.0429	3.2206	3.2206	2.5434
1.5	1.5	3.6725	3.6725	3.6725	3.6725	3.6725	3.6725	3.6725	3.6725	3.6725
1.5	2.0	6.0458	6.0458	10.7481	4.4580	4.4580	7.9254	6.3144	6.3144	11.2255
1.5	2.5	8.6261	8.6261	23.9614	6.8533	6.8533	19.0368	10.4359	10.4359	28.9887
1.5	3.0	11.2295	11.2295	44.9178	10.3536	10.3536	41.4143	15.4728	15.4728	61.8913
1.5	4.0	16.0441	16.0441	114.0913	18.9646	18.9646	134.8595	26.5208	26.5208	188.5926
1.5	6.0	23.1266	23.1266	370.0260	35.9359	35.9359	574.9741	46.2619	46.2619	740.1909

**Table G.6:** Scalings of cross section times BR for the non-resolved model, for the different  $t\bar{t}H$ ,  $tHq$ ,  $tHW$  signal components and  $\kappa_V = 1.5$ .

$\cos(\alpha_{CP})$	Exp.	SM exp.	Obs.	Best fit $\sigma[pb]$ .	Best fit r
-1.0	0.299 <sup>0.130</sup> <sub>-0.088</sub>	0.396 <sup>0.190</sup> <sub>-0.135</sub>	0.594	0.284 <sup>0.183</sup> <sub>-0.171</sub>	0.650 <sup>0.418</sup> <sub>-0.391</sub>
-0.9	0.297 <sup>0.130</sup> <sub>-0.088</sub>	0.388 <sup>0.184</sup> <sub>-0.132</sub>	0.578	0.268 <sup>0.182</sup> <sub>-0.171</sub>	0.686 <sup>0.466</sup> <sub>-0.438</sub>
-0.8	0.294 <sup>0.129</sup> <sub>-0.088</sub>	0.377 <sup>0.179</sup> <sub>-0.127</sub>	0.562	0.251 <sup>0.181</sup> <sub>-0.171</sub>	0.725 <sup>0.522</sup> <sub>-0.493</sub>
-0.7	0.292 <sup>0.129</sup> <sub>-0.087</sub>	0.377 <sup>0.165</sup> <sub>-0.132</sub>	0.545	0.235 <sup>0.179</sup> <sub>-0.170</sub>	0.768 <sup>0.587</sup> <sub>-0.556</sub>
-0.6	0.288 <sup>0.128</sup> <sub>-0.086</sub>	0.368 <sup>0.155</sup> <sub>-0.128</sub>	0.523	0.215 <sup>0.177</sup> <sub>-0.169</sub>	0.798 <sup>0.638</sup> <sub>-0.627</sub>
-0.5	0.285 <sup>0.127</sup> <sub>-0.086</sub>	0.365 <sup>0.166</sup> <sub>-0.132</sub>	0.500	0.194 <sup>0.176</sup> <sub>-0.167</sub>	0.813 <sup>0.739</sup> <sub>-0.701</sub>
-0.4	0.281 <sup>0.126</sup> <sub>-0.085</sub>	0.357 <sup>0.150</sup> <sub>-0.128</sub>	0.479	0.175 <sup>0.174</sup> <sub>-0.165</sub>	0.840 <sup>0.833</sup> <sub>-0.792</sub>
-0.3	0.279 <sup>0.125</sup> <sub>-0.084</sub>	0.350 <sup>0.150</sup> <sub>-0.125</sub>	0.463	0.162 <sup>0.173</sup> <sub>-0.162</sub>	0.884 <sup>0.943</sup> <sub>-0.884</sub>
-0.2	0.277 <sup>0.124</sup> <sub>-0.084</sub>	0.346 <sup>0.153</sup> <sub>-0.117</sub>	0.453	0.153 <sup>0.172</sup> <sub>-0.153</sub>	0.954 <sup>0.968</sup> <sub>-0.954</sub>
-0.1	0.277 <sup>0.124</sup> <sub>-0.084</sub>	0.345 <sup>0.155</sup> <sub>-0.123</sub>	0.454	0.154 <sup>0.171</sup> <sub>-0.154</sub>	1.075 <sup>1.197</sup> <sub>-1.075</sub>
0.0	0.279 <sup>0.125</sup> <sub>-0.084</sub>	0.353 <sup>0.161</sup> <sub>-0.130</sub>	0.469	0.167 <sup>0.173</sup> <sub>-0.164</sub>	1.304 <sup>1.356</sup> <sub>-1.282</sub>
0.1	0.285 <sup>0.127</sup> <sub>-0.086</sub>	0.371 <sup>0.160</sup> <sub>-0.137</sub>	0.504	0.197 <sup>0.177</sup> <sub>-0.167</sub>	1.683 <sup>1.508</sup> <sub>-1.427</sub>
0.2	0.293 <sup>0.129</sup> <sub>-0.087</sub>	0.390 <sup>0.159</sup> <sub>-0.143</sub>	0.556	0.246 <sup>0.180</sup> <sub>-0.171</sub>	2.234 <sup>1.639</sup> <sub>-1.552</sub>
0.3	0.300 <sup>0.130</sup> <sub>-0.089</sub>	0.416 <sup>0.178</sup> <sub>-0.152</sub>	0.610	0.303 <sup>0.182</sup> <sub>-0.171</sub>	2.860 <sup>1.723</sup> <sub>-1.612</sub>
0.4	0.302 <sup>0.129</sup> <sub>-0.088</sub>	0.422 <sup>0.193</sup> <sub>-0.143</sub>	0.644	0.349 <sup>0.177</sup> <sub>-0.166</sub>	3.331 <sup>1.693</sup> <sub>-1.587</sub>
0.5	0.296 <sup>0.125</sup> <sub>-0.086</sub>	0.434 <sup>0.157</sup> <sub>-0.145</sub>	0.651	0.374 <sup>0.165</sup> <sub>-0.159</sub>	3.452 <sup>1.527</sup> <sub>-1.467</sub>
0.6	0.284 <sup>0.120</sup> <sub>-0.082</sub>	0.425 <sup>0.136</sup> <sub>-0.141</sub>	0.639	0.377 <sup>0.155</sup> <sub>-0.150</sub>	3.261 <sup>1.339</sup> <sub>-1.298</sub>
0.7	0.270 <sup>0.114</sup> <sub>-0.078</sub>	0.408 <sup>0.118</sup> <sub>-0.133</sub>	0.616	0.366 <sup>0.147</sup> <sub>-0.140</sub>	2.910 <sup>1.167</sup> <sub>-1.111</sub>
0.8	0.258 <sup>0.109</sup> <sub>-0.074</sub>	0.386 <sup>0.120</sup> <sub>-0.120</sub>	0.594	0.354 <sup>0.141</sup> <sub>-0.132</sub>	2.530 <sup>1.006</sup> <sub>-0.945</sub>
0.9	0.246 <sup>0.104</sup> <sub>-0.071</sub>	0.358 <sup>0.128</sup> <sub>-0.105</sub>	0.570	0.341 <sup>0.135</sup> <sub>-0.126</sub>	2.161 <sup>0.857</sup> <sub>-0.798</sub>
1.0	0.238 <sup>0.101</sup> <sub>-0.069</sub>	0.351 <sup>0.125</sup> <sub>-0.101</sub>	0.555	0.331 <sup>0.132</sup> <sub>-0.121</sub>	1.851 <sup>0.736</sup> <sub>-0.679</sub>

**Table G.7:** Expected (for background only, and for a SM-like Higgs signal) and observed 95% C.L. upper limits (in pb), and best fit signal strength  $r$  and corresponding best fit cross section for the combined  $tH + t\bar{t}H$  cross section times branching ratio for the combination of all three channels, for different values of  $\cos(\alpha_{CP})$ .

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