

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.

4 by

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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>321</sup> Chapter 1

## <sup>322</sup> Theoretical approach

### <sup>323</sup> 1.1 Introduction

<sup>324</sup> The physical description of the universe is a challenge that physicists have faced by  
<sup>325</sup> making theories that refine existing principles and proposing new ones in an attempt  
<sup>326</sup> to embrace emerging facts and phenomena.

<sup>327</sup> At the end of 1940s Julian Schwinger [1] and Richard P. Feynman [2], based on  
<sup>328</sup> the work of Sin-Itiro Tomonaga [3], developed an electromagnetic theory consistent  
<sup>329</sup> with special relativity and quantum mechanics that describes how matter and light  
<sup>330</sup> interact; the so-called *quantum electrodynamics* (QED) was born.

<sup>331</sup> QED has become the blueprint for developing theories that describe the universe.  
<sup>332</sup> It was the first example of a quantum field theory (QFT), which is the theoretical  
<sup>333</sup> framework for building quantum mechanical models that describes particles and their  
<sup>334</sup> interactions. QFT is composed of a set of mathematical tools that combines classical  
<sup>335</sup> fields, special relativity and quantum mechanics, while keeping the quantum point  
<sup>336</sup> particles and locality ideas.

<sup>337</sup> This chapter gives an overview of the standard model of particle physics, starting

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

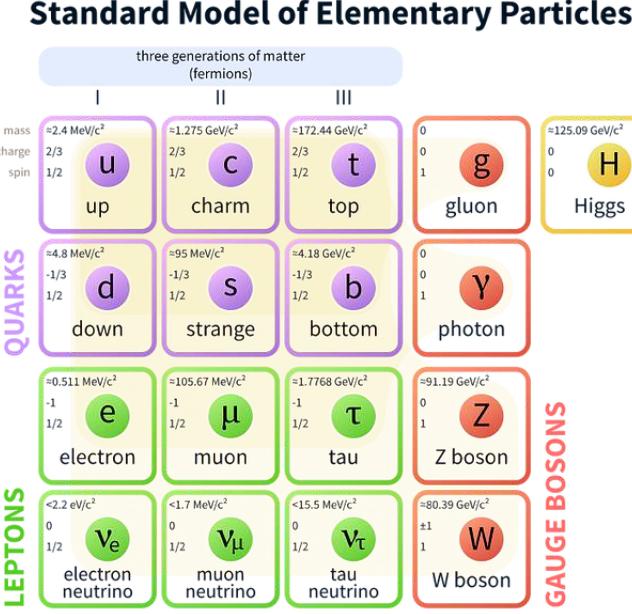
## 342 1.2 Standard model of particle physics

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

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

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

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

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

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

373 **1.2.1 Fermions**

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

379

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

387 first and second generation fermions is small compared to the mass difference with  
 388 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.

389

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

392 **1.2.1.1 Leptons**

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

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

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

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

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

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

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

425 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.

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

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

437

### 438 1.2.1.2 Quarks

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

443

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

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

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

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

464 In the first version of the quark model (1964), M. Gell-Mann [12] and G. Zweig  
 465 [13, 14] developed a consistent way to classify hadrons according to their properties.  
 466 Only three quarks (u, d, s) were involved in a scheme in which all baryons have baryon  
 467 number  $B=1$  and therefore quarks have  $B=1/3$ ; non-baryons have  $B=0$ . Baryon  
 468 number is conserved in SI and EI which means that single quarks cannot be created  
 469 but in pairs  $q - \bar{q}$ .

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

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

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

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

477

478 Isospin doublets of quarks are also defined (see Table 1.5), and same as for neutrinos,  
 479 the WI eigenstates are not the same as the mass eigenstates which means that  
 480 members of different quark generations are connected by the WI mediator; thus, up-  
 481 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:

484

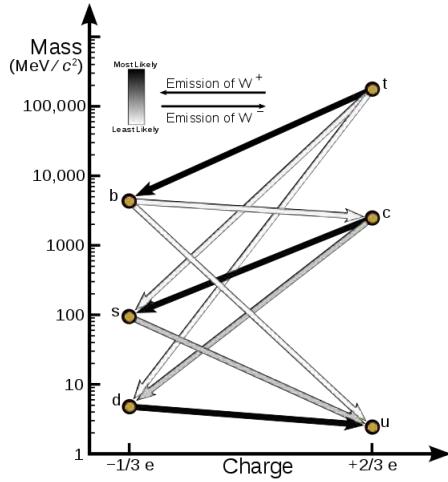
$$\begin{aligned} q'_d &= V_{CKM} q_d \\ \begin{pmatrix} d' \\ s' \\ b' \end{pmatrix} &= \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix} \end{aligned} \quad (1.3)$$

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

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

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

491 CKM matrix is a  $3 \times 3$  unitary matrix parametrized by three mixing angles and  
 492 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].

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

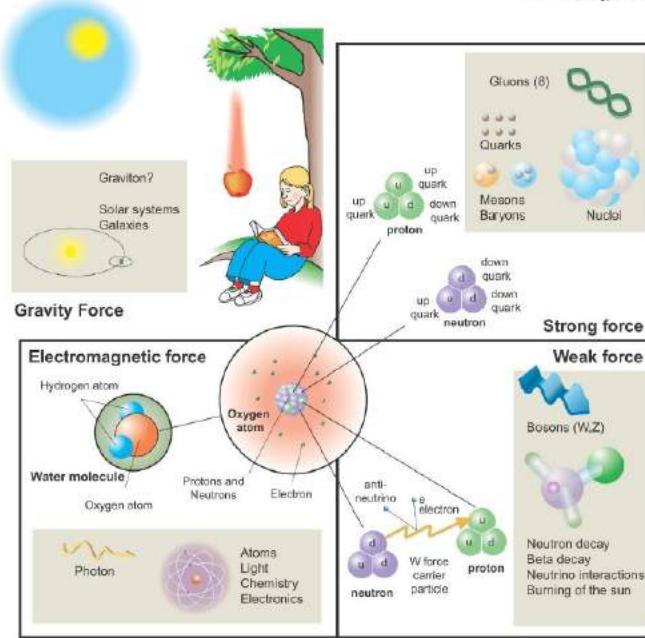
### 497 1.2.2 Fundamental interactions

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

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

## Fundamental interactions.

Illustration: Typoform



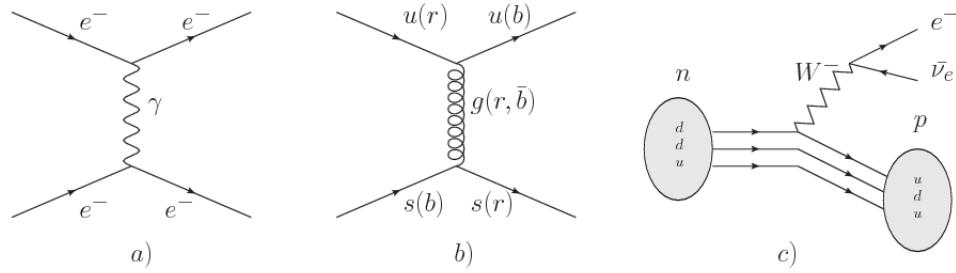
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**Figure 1.3:** Fundamental interactions in nature. Despite the many manifestations of forces in nature, we can track all of them back to one of the fundamental interactions. The most common forces are gravity and electromagnetic given that all of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

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

- 513 • *Weak interaction (WI)* described by the weak theory (WT), is responsible, for  
 514 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

533 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].

534

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

549 **1.2.3 Gauge invariance.**

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

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

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

571     When the gauge transformation:

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

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

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

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

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

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

#### 601 1.2.4 Gauge bosons

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

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

- 616     • **Gluon.** SI is mediated by gluons which just as photons are massless. They  
 617       carry one unit of color charge and one unit of anticolor charge, hence, gluons  
 618       can couple to other gluons. As a result, the range of the SI is not infinite  
 619       but very short due to the attraction between gluons, giving rise to the *color*  
 620       *confinement* which explains why color charged particles cannot be isolated but  
 621       live within composite particles, like quarks inside protons.
- 622     • **W, Z.**  $W^\pm$  and Z, are massive which explains their short-range. Given that  
 623       the WI is the only interaction that can change the flavor of the interacting  
 624       particles, the W boson is the responsible for the nuclear transmutation where  
 625       a neutron is converted into a proton or vice versa with the involvement of an  
 626       electron and a neutrino (see Figure 1.4c). The Z boson is the responsible for the  
 627       neutral weak processes like neutrino elastic scattering where no electric charge  
 628       but momentum transference is involved. WI gauge bosons carry isospin charge  
 629       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	$91.188 \pm 0.002$

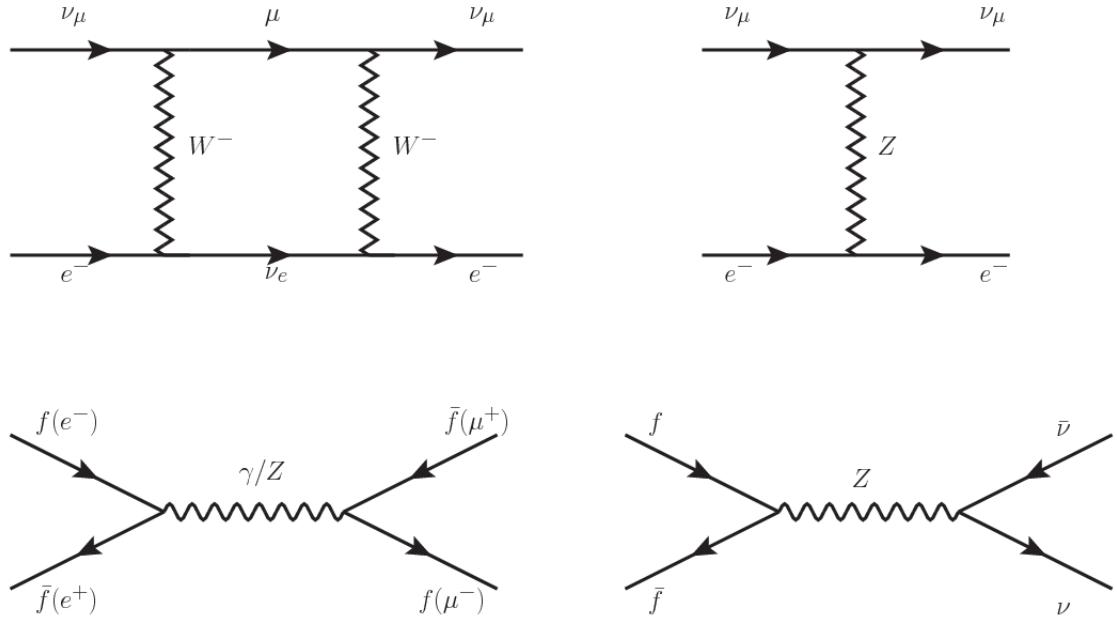
**Table 1.7:** SM gauge bosons main features [9].

630

### 631    1.3 Electroweak unification and the Higgs 632       mechanism

633    Physicists dream of building a theory that contains all the interactions in one single  
 634    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

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

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

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

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

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

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

671 Given the first generation of leptons

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

672 the charged fermionic currents are given by

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

673 and the free Lagrangian is given by

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

724 The neutral gauge fields  $W_\mu^3$  and  $B_\mu$  cannot be directly identified with the  $Z$   
 725 and the photon fields since the photon interacts similarly with left and right-handed  
 726 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

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

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

728 electromagnetic interaction under the condition

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

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

730

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

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

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

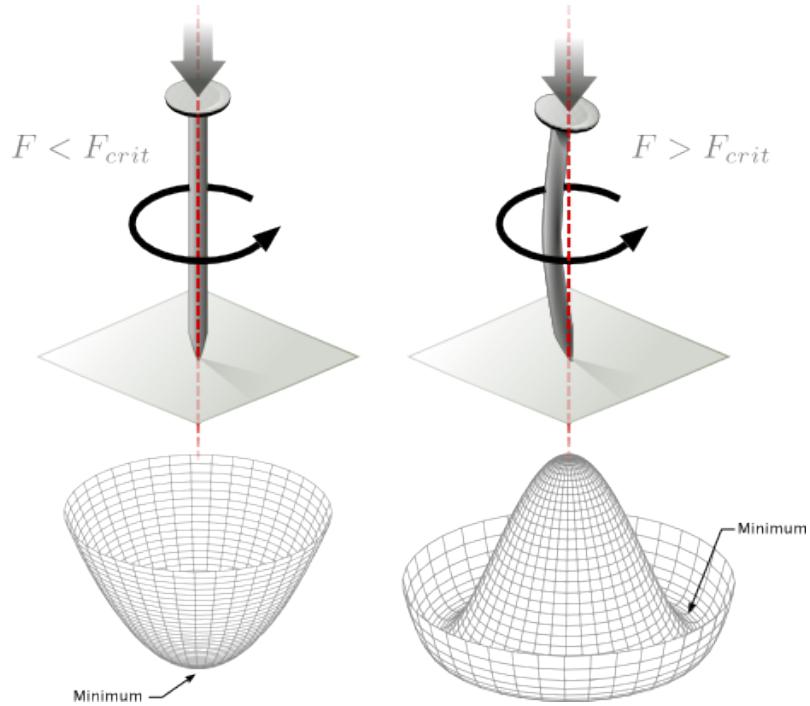
$$\mathcal{L}_{nmEWI} = \mathcal{L}_0 + \mathcal{L}_G \quad (1.30)$$

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

### 739 1.3.1 Spontaneous symmetry breaking (SSB)

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

742 Before reaching the critical force value, the system has rotational symmetry with  
 743 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].

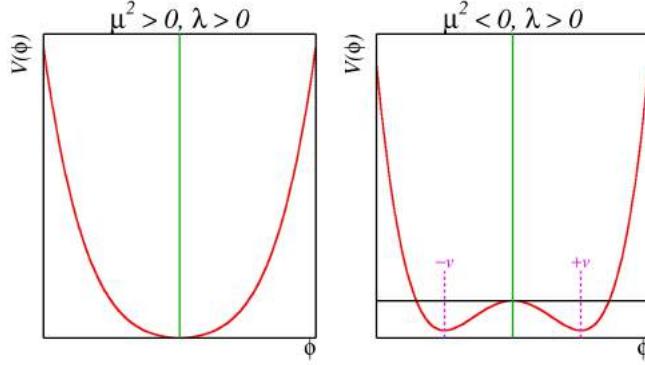
744 les (top right). The form of the potential energy (bottom right) changes appearing a  
 745 set of infinity minima but preserving its rotational symmetry. Right before the nail  
 746 buckles there is no indication of the direction the nail will bend because any of the  
 747 directions are equivalent,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

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

753 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  $\phi(x)$

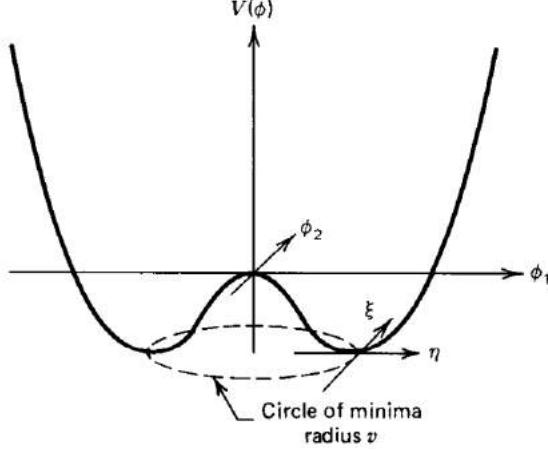
$$\phi(x) = \frac{1}{\sqrt{2}}(\phi_1 + i\phi_2) \quad (1.32)$$

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].

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

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

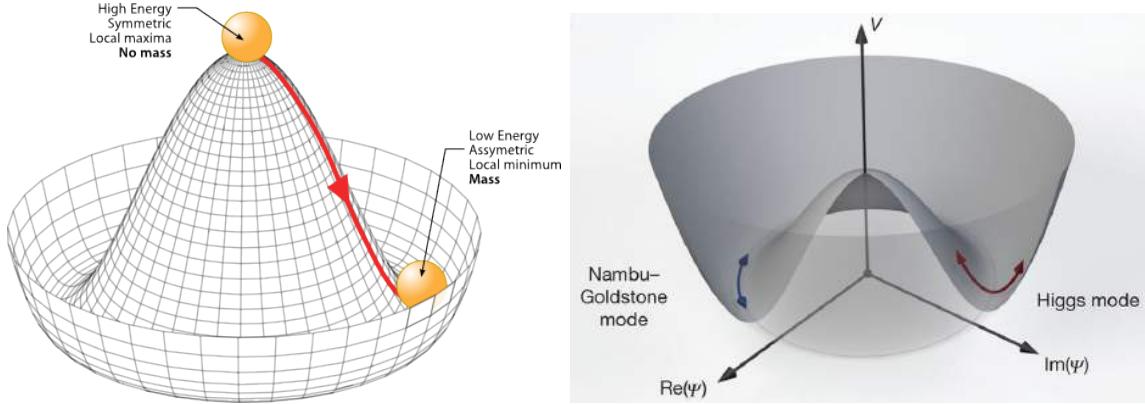
$$\phi(x) = \frac{1}{\sqrt{2}}(v + \eta(x) + i\xi(x)) \quad (1.35)$$

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

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

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

770 present in the system; after the SSB there are two fields of which the  $\eta$ -field has  
 771 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].

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

### 782 1.3.2 Higgs mechanism

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

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

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

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

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

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

790 The minima of the potential are defined by

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

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

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

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

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

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

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

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

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

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

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

819 **1.3.3 Masses of the gauge bosons**

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

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

822 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

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

823 and then

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

824 **1.3.4 Masses of the fermions**

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

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

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

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

829

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

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

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

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

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

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

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

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

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

### 841 1.3.5 The Higgs field

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

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

845

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

846

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

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

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

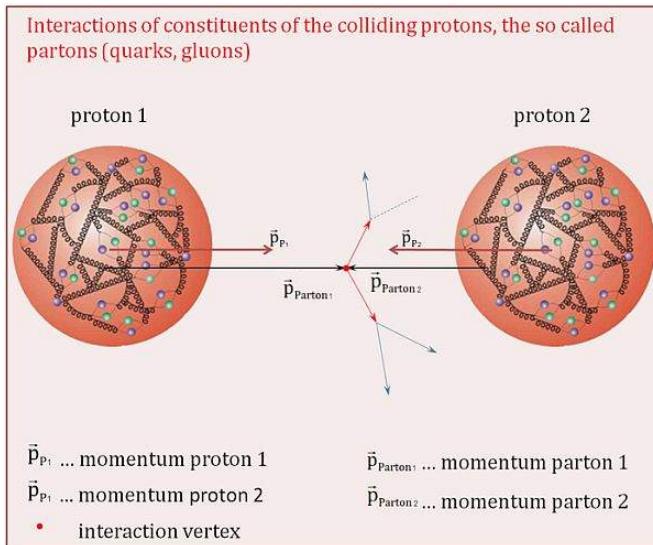
849 however, it is not predicted by the theory either. The experimental measurement of  
850 the Higgs boson mass have been performed by the *Compact Muon Solenoid (CMS)*  
851 experiment and the *A Toroidal LHC Appartus (ATLAS)* experiments at the *Large  
852 Hadron Collider(LHC)*, [36–38], and is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

### 854 1.3.6 Production of Higgs bosons at LHC

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



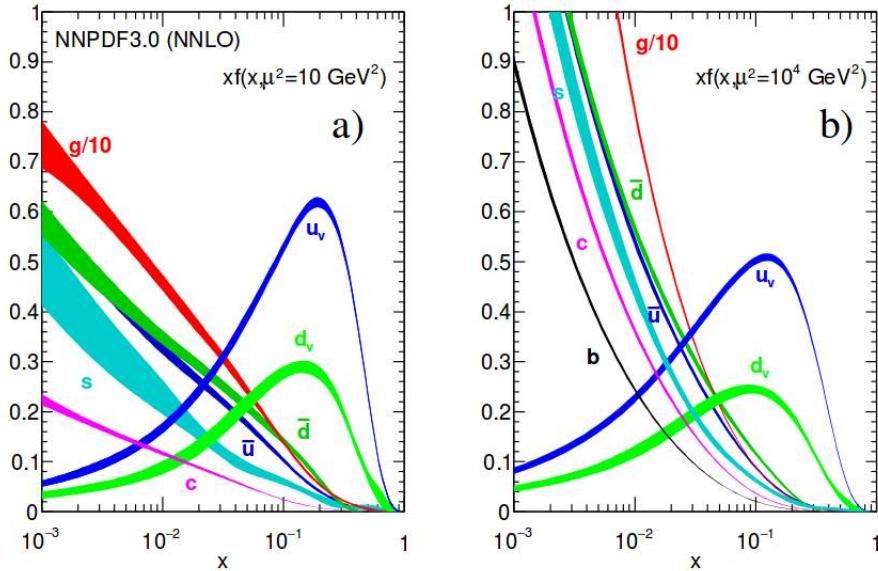
**Figure 1.10:** Proton-proton collision. Protons are composed of 3 valence quarks, a sea of quarks and gluons; therefore in a proton-proton collision, quarks and gluons are those who collide. [39].

857

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

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

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

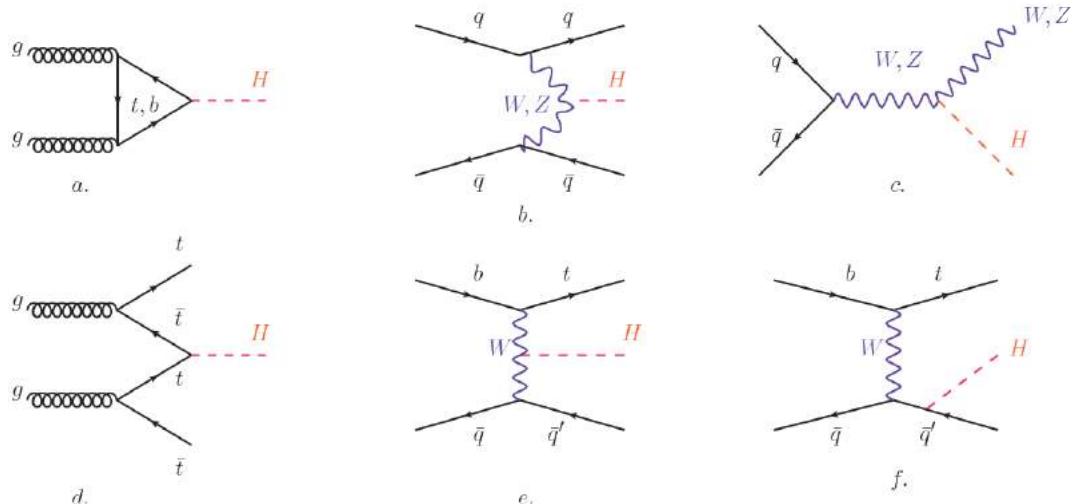


**Figure 1.11:** Proton PDFs for two values of  $Q^2$ : left.  $\mu^2 = Q^2 = 10 \text{ GeV}^2$ , right.  $\mu^2 = Q^2 = 10^4 \text{ GeV}^2$ .  $u_v$  and  $d_v$  correspond to the  $u$  and  $d$  valence quarks,  $s, c, b, \bar{u}, \bar{d}$  correspond to sea quarks, and  $g$  corresponds to gluons.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

873 In physics, a common approach to study complex systems consists of starting  
 874 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.

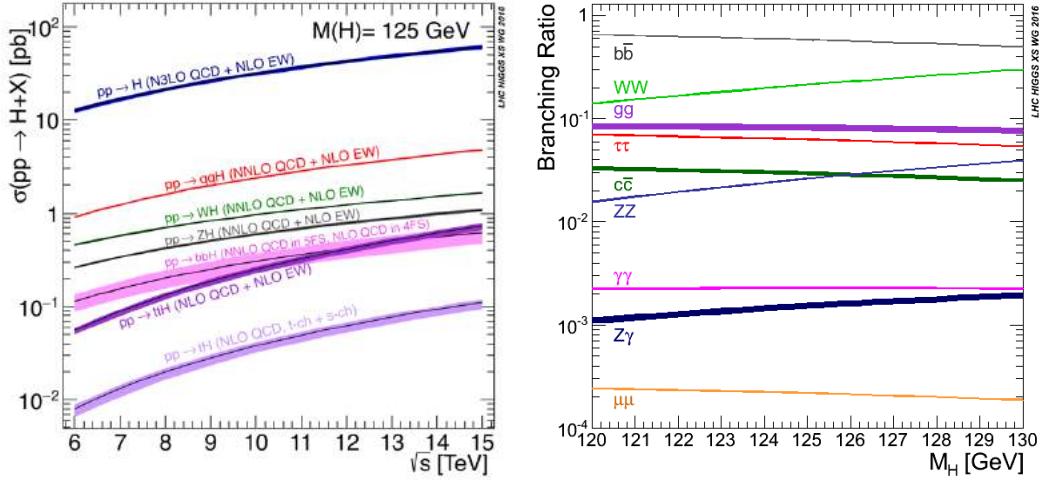
High energy systems, like the Higgs production at LHC explored in this thesis, usually can be treated perturbatively with the expansion made in terms of the coupling constants. The overview presented here will be oriented specifically to the Higgs boson production mechanisms in  $pp$  collisions at LHC.



**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

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

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

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

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

### 922 1.3.7 Higgs boson decay channels

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

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

932

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

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

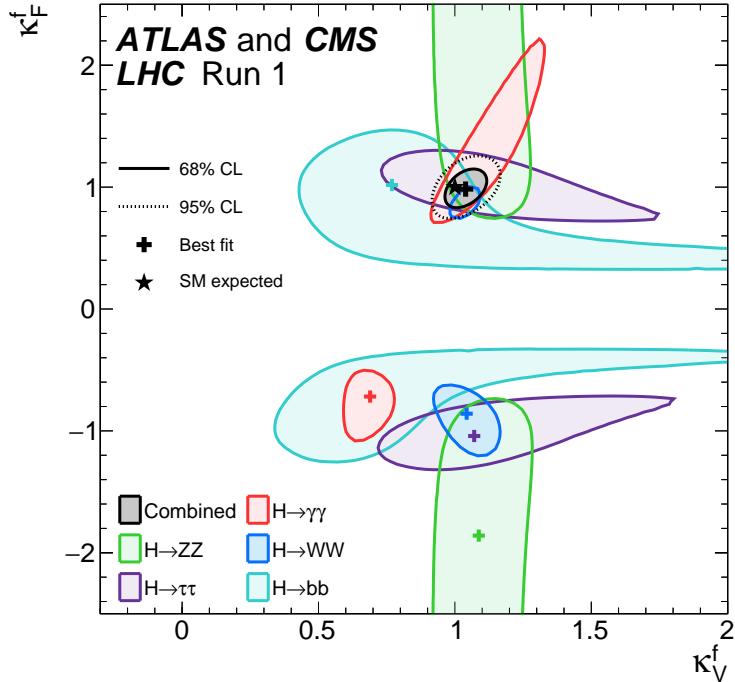
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<sup>8</sup> In general, on-shell or real particles are those which satisfy the energy-momentum relation ( $E^2 - |\vec{p}|^2 c^2 = m^2 c^4$ ); off-shell or virtual particles does not satisfy it which is possible under the uncertainty principle of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

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

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

949 **1.4 Experimental status of the anomalous  
 950 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].

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

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

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

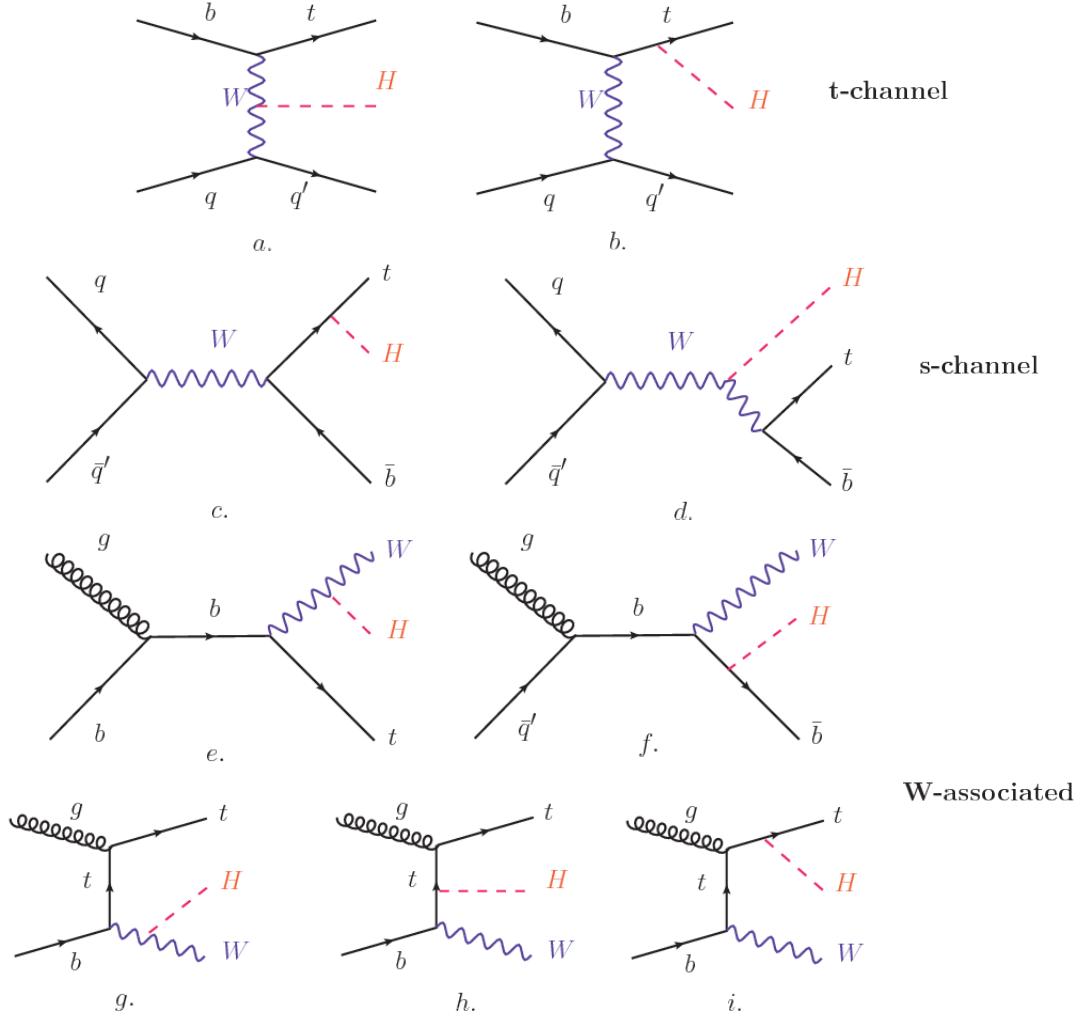
977 of the H-t coupling and the access to information from the Higgs boson production  
 978 rather than from its decays.

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

## 984 **1.5 Associated production of a Higgs boson and a 985 single top quark**

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

1013 emission of an approximately on-shell W and its hard scattering with the b quark;  
 1014 i.e.  $Wb \rightarrow th$ . The scattering amplitude for the process is given by

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

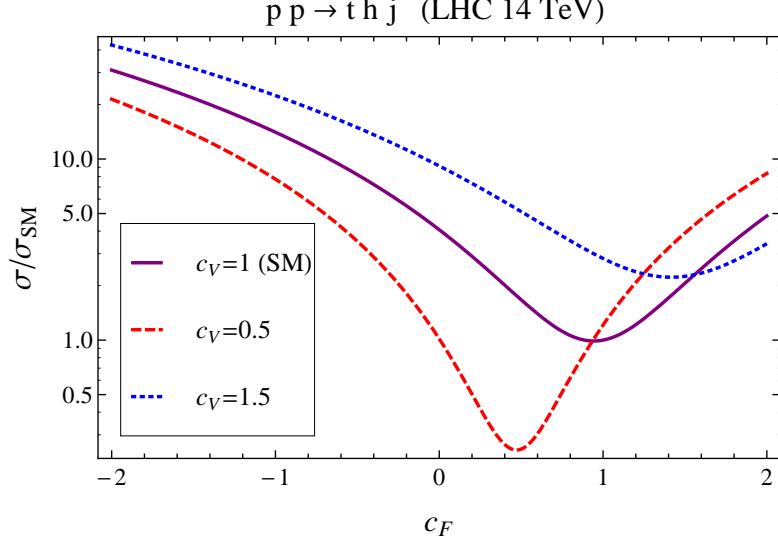
1015 where  $\kappa_V \equiv g_{HVV}/g_{HVV}^{SM}$  and  $\kappa_t \equiv g_{Ht}/g_{Ht}^{SM} = y_t/y_t^{SM}$  are scaling factors that quantify  
 1016 possible deviations of the couplings from the SM values, Higgs-Vector boson (H-  
 1017 W) and Higgs-top (H-t) respectively, from the SM couplings;  $s = (p_W + p_b)^2$ ,  $t =$   
 1018  $(p_W - p_H)^2$ ,  $\varphi$  is the Higgs azimuthal angle around the  $z$  axis taken parallel to the  
 1019 direction of motion of the incoming W; A and B are functions describing the weak  
 1020 interaction in terms of the chiral states  $(\xi_t, \xi_b)$  of the quarks  $b$  and  $t$ . Terms that  
 1021 vanish in the high energy limit have been neglected as well as the Higgs and  $b$  quark  
 1022 masses<sup>9</sup>.

1023 The scattering amplitude grows with energy like  $\sqrt{s}$  for  $\kappa_V \neq \kappa_t$ , in contrast to  
 1024 the SM ( $\kappa_t = \kappa_V = 1$ ), where the first term in 1.62 cancels out and the amplitude  
 1025 is constant for large  $s$ ; therefore, a deviation from the SM predictions represents an  
 1026 enhancement in the  $tHq$  cross section. In particular, for a SM H-W coupling and a  
 1027 H-t coupling of inverted sign with respect to the SM ( $\kappa_V = -\kappa_t = 1$ ) the  $tHq$  cross  
 1028 section is enhanced by a factor greater 10 as seen in the Figure 1.16 taken from  
 1029 Reference [51]; Reference [56] has reported similar enhancement results.

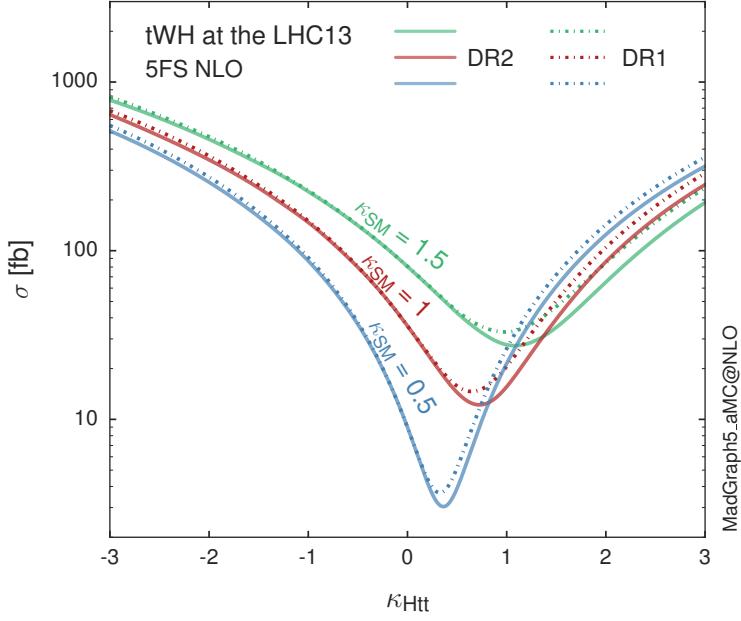
1030 A similar analysis is valid for the W-associated channel but, in that case, the in-  
 1031 terference is more complicated since there are more than two contributions and an ad-  
 1032 ditional interference with the production of Higgs boson and a top pair process( $t\bar{t}H$ ).  
 1033 The calculations 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.

1042

## 1043 1.6 CP-mixing in $tH$ processes

1044 In addition to the sensitivity to sign of the H-t coupling, the  $tHq$  and  $tHW$  processes  
 1045 have been proposed as a tool to investigate the possibility of a H-t coupling that does

1046 not conserve CP [47, 48, 58].

1047 In this thesis, the sensitivity of  $tH$  processes to CP-mixing is also studied on the  
 1048 basis of References [47, 48] using the effective field theory framework where a generic  
 1049 particle ( $X_0$ ) of spin-0 and a general CP violating interaction with the top quark  
 1050 ( $Htt$  coupling), can couple to scalar and pseudo-scalar fermionic densities. The H-W  
 1051 interaction is assumed to be SM-like. The Lagrangian modeling the H-t interaction  
 1052 is given by

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

1053 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  
 1054 dimensionless re-scaling parameters<sup>10</sup> used to parametrize the magnitude of the CP-  
 1055 violating and CP-conserving parts of the amplitude. The model defines  $g_{Htt} =$   
 1056  $g_{Att} = m_t/v = y_t/\sqrt{2}$  with  $v \sim 246$  GeV the Higgs vacuum expectation value. In  
 1057 this parametrization, three special cases can be recovered

1058 • CP-even coupling  $\rightarrow \alpha = 0^\circ$

1059 • CP-odd coupling  $\rightarrow \alpha = 90^\circ$

1060 • SM coupling  $\rightarrow \alpha = 0^\circ$  and  $\kappa_{Htt} = 1$

1061 The loop induced  $X_0$  coupling to gluons can also be described in terms of the  
 1062 parametrization above, according to

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

1063 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.

1064 Under the assumption that the top quark dominates the gluon-fusion process at LHC

---

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

1065 energies,  $\kappa_{Hgg} \rightarrow \kappa_{Htt}$  and  $\kappa_{Agg} \rightarrow \kappa_{Att}$ , so that the ratio between the gluon-gluon  
 1066 fusion cross section for  $X_0$  and for the SM Higgs prediction can be written as

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

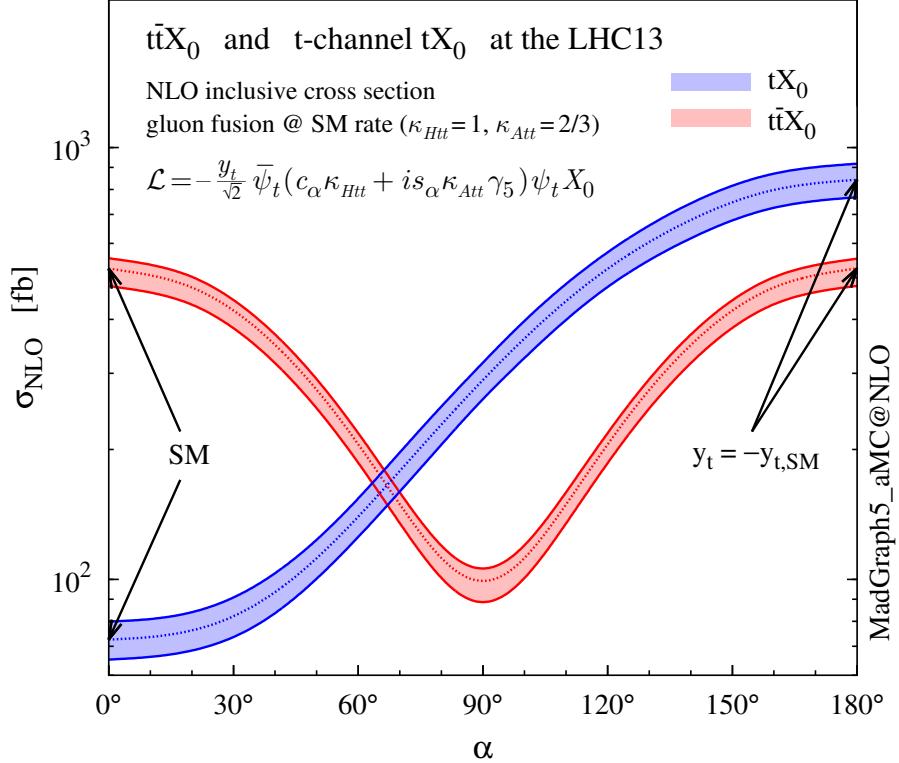
1067 If the re-scaling parameters are set to

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

1068 the gluon-fusion SM cross section is reproduced for every value of the CP-mixing  
 1069 angle  $\alpha$ ; therefore, by imposing that condition to the Lagrangian density 1.63, the  
 1070 CP-mixing angle is not constrained by current data. Figure 1.18 shows the NLO cross  
 1071 sections for t-channel  $tX_0$ (blue) and  $t\bar{t}X_0$  (red) associated production processes as a  
 1072 function of the CP-mixing angle  $\alpha$ .  $X_0$  is a generic spin-0 particle with top quark  
 1073 CP-violating coupling. Re-scaling factors  $\kappa_{Htt}$  and  $\kappa_{Att}$  have been set to reproduce  
 1074 the SM gluon-fusion cross sections.

1075 It is interesting to notice that the  $tX_0$  cross section is enhanced, by a factor of  
 1076 about 10, when a continuous rotation in the scalar-pseudoscalar plane is applied; this  
 1077 enhancement is similar to the enhancement produced when the H-t coupling is flipped  
 1078 in sign with respect to the SM ( $y_t = -y_{t,SM}$  in the plot), as showed in Section 1.5. In  
 1079 contrast, the degeneracy in the  $t\bar{t}X_0$  cross section is still present given that it depends  
 1080 quadratically on the H-t coupling, but more interesting is to notice that  $t\bar{t}X_0$  cross  
 1081 section is exceeded by  $tX_0$  cross section after  $\alpha \sim 60^\circ$ .

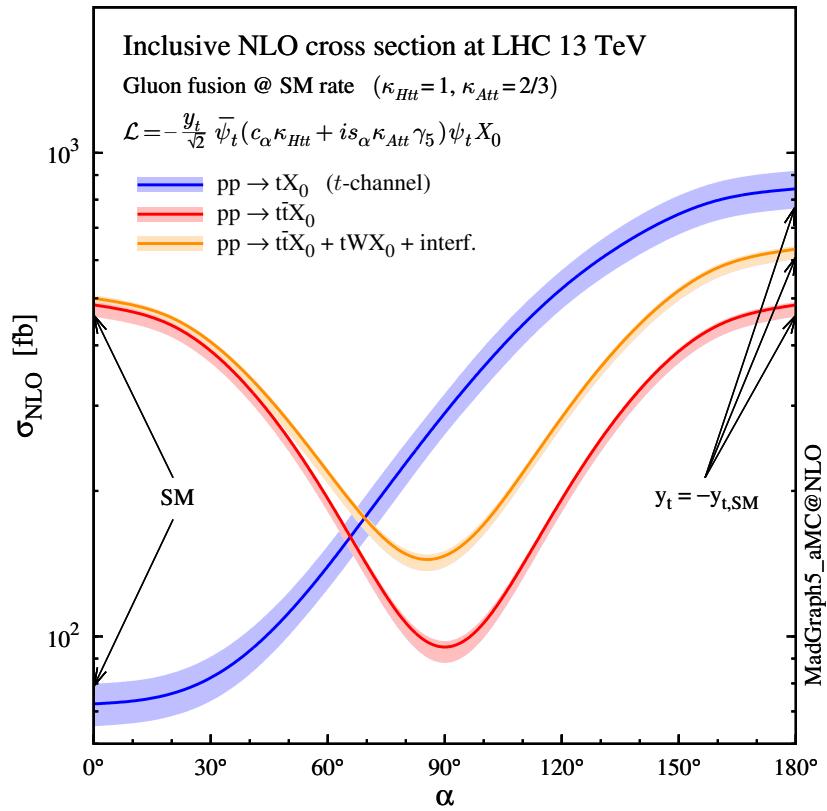
1082 A similar parametrization can be used to investigate the  $tHW$  process sensitivity  
 1083 to CP-violating H-t coupling. As said in 1.5, the interference in the W-associated  
 1084 channel is more complicated because there are more than two contributions and also  
 1085 there is interference 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].

1086       Figure 1.19 shows the NLO cross sections for t-channel  $tX_0$ (blue),  $t\bar{t}X_0$  (red)  
 1087       associated production and for the combined  $tWX_0+t\bar{t}X_0+interference$  (orange) as  
 1088       a function of the CP-mixing angle. It is clear that the effect of the interference in the  
 1089       combined case is the lifting of the degeneracy present in the  $t\bar{t}X_0$  production. The  
 1090       constructive interference enhances the cross section from about 500 fb at SM ( $\alpha = 0$ )  
 1091       to about 600 fb ( $\alpha = 180^\circ \rightarrow y_t = -y_{t,SM}$ ).

1092       An analysis combining  $tHq$  and  $tHW$  processes will be made in this thesis taking  
 1093       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>1094</sub> **Chapter 2**

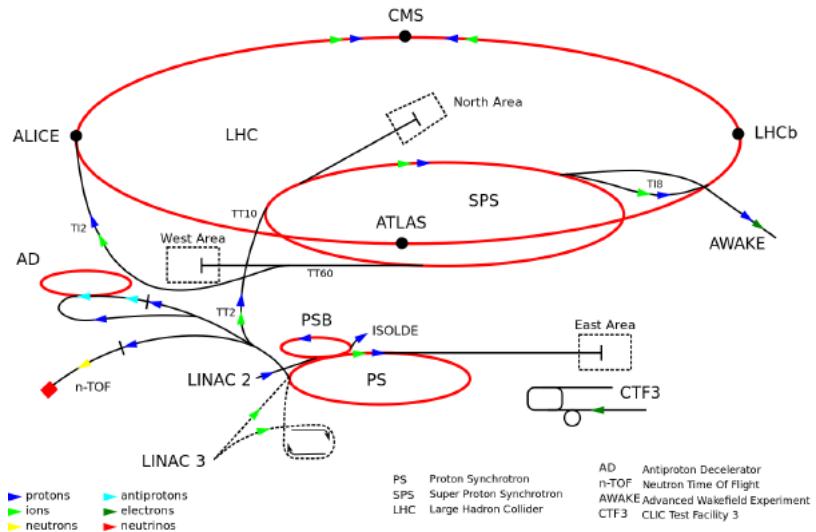
<sub>1095</sub> **The CMS experiment at the LHC**

<sub>1096</sub> **2.1 Introduction**

<sub>1097</sub> Located on the Swiss-French border, the European Council for Nuclear Research  
<sub>1098</sub> (CERN) is the largest scientific organization leading particle physics research. About  
<sub>1099</sub> 13000 people in a broad range of roles including users, students, scientists, engineers,  
<sub>1100</sub> among others, contribute to the data taking and analysis, with the goal of unveiling  
<sub>1101</sub> the secrets of nature and revealing the fundamental structure of the universe. CERN  
<sub>1102</sub> is also the home of the Large Hadron Collider (LHC), the largest particle accelerator  
<sub>1103</sub> around the world, where protons (or heavy ions) traveling close to the speed of light,  
<sub>1104</sub> are made to collide. These collisions open a window to investigate how particles (and  
<sub>1105</sub> their constituents if they are composite) interact with each other, providing clues  
<sub>1106</sub> about the laws of nature. This chapter presents an overview of the LHC structure  
<sub>1107</sub> and operation. A detailed description of the CMS detector is offered, given that the  
<sub>1108</sub> data used in this thesis have been taken with this detector.

## 1109 2.2 The LHC

1110 With 27 km of circumference, the LHC is currently the most powerful circular accelerator  
 1111 in the world. It is installed in the same tunnel where the Large Electron-Positron  
 1112 (LEP) collider was located, taking advantage of the existing infrastructure. The LHC  
 1113 is part of the CERN's accelerator complex composed of several successive accelerat-  
 1114 ing stages before the particles are injected into the LHC ring where they reach their  
 1115 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].

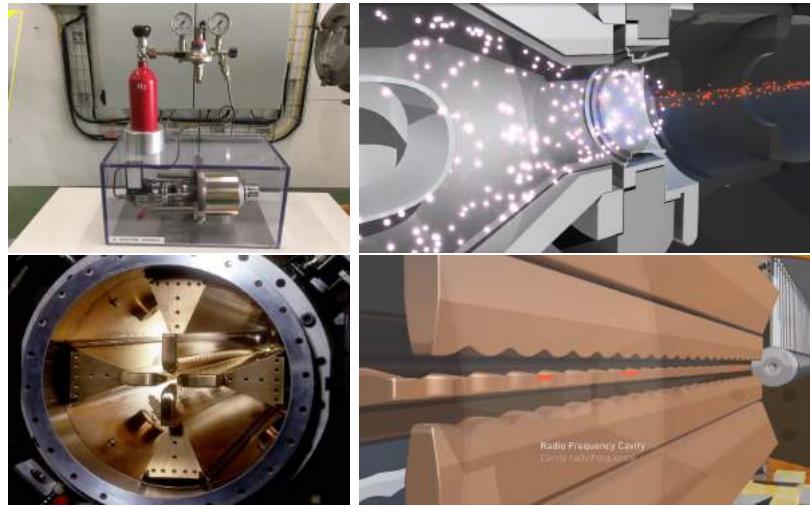
1116 The LHC runs in three collision modes depending on the particles being acceler-  
 1117 ated

1118 • Proton-Proton collisions ( $pp$ ) for multiple physics experiments.

1119 • Lead-Lead collisions ( $Pb-Pb$ ) for heavy ion experiments.

1120 • Proton-Lead collisions ( $p-Pb$ ) for quark-gluon plasma experiments.

1121 In this thesis only  $pp$  collisions will be considered.

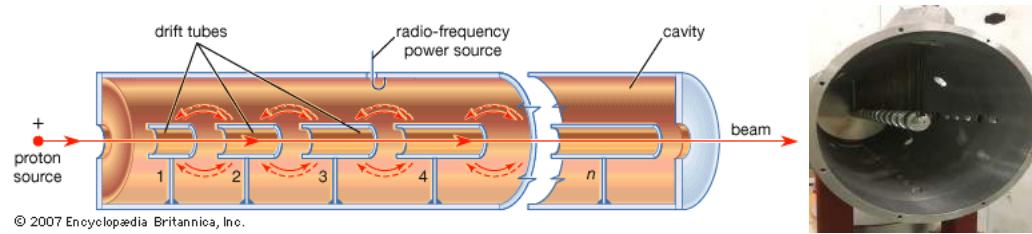


**Figure 2.2:** LHC protons source and the first acceleration stage. Top: the bottle contains hydrogen gas which is injected into the metal cylinder (white dots) to be broken down into electrons (blue dots) and protons (red dots); Bottom: the obtained protons are directed towards the radio frequency 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].

1122 Collection of protons starts with hydrogen atoms taken from a bottle, containing  
 1123 hydrogen gas, and injecting them in a metal cylinder; hydrogen atoms are broken  
 1124 down into electrons and protons by an intense electric field (see Figure 2.2 top).  
 1125 The resulting protons leave the metal cylinder towards a radio frequency quadrupole  
 1126 (RFQ) that focus the beam, accelerates the protons and creates the packets of protons  
 1127 called bunches. In the RFQ, an electric field is generated by a RF wave at a frequency  
 1128 that matches the resonance frequency of the cavity where the electrodes are contained.  
 1129 The beam of protons traveling on the RFQ axis experiences an alternating electric  
 1130 field gradient that generates the focusing forces.

1131 In order to accelerate the protons, a longitudinal time-varying electric field com-  
 1132 ponent is added to the system; it is done by giving the electrodes a sine-like profile as  
 1133 shown in Figure 2.2 bottom. By matching the speed and phase of the protons with  
 1134 the longitudinal electric field the bunching is performed; protons synchronized with

1135 the RFQ (synchronous protons) do not feel an accelerating force, but those protons in  
 1136 the beam that have more (or less) energy than the synchronous proton (asynchronous  
 1137 protons) will feel a decelerating (accelerating) force; therefore, asynchronous protons  
 1138 will oscillate around the synchronous ones forming bunches of protons [63]. From the  
 1139 RFQ protons emerge with energy 750 keV in bunches of about  $1.15 \times 10^{11}$  protons [64].

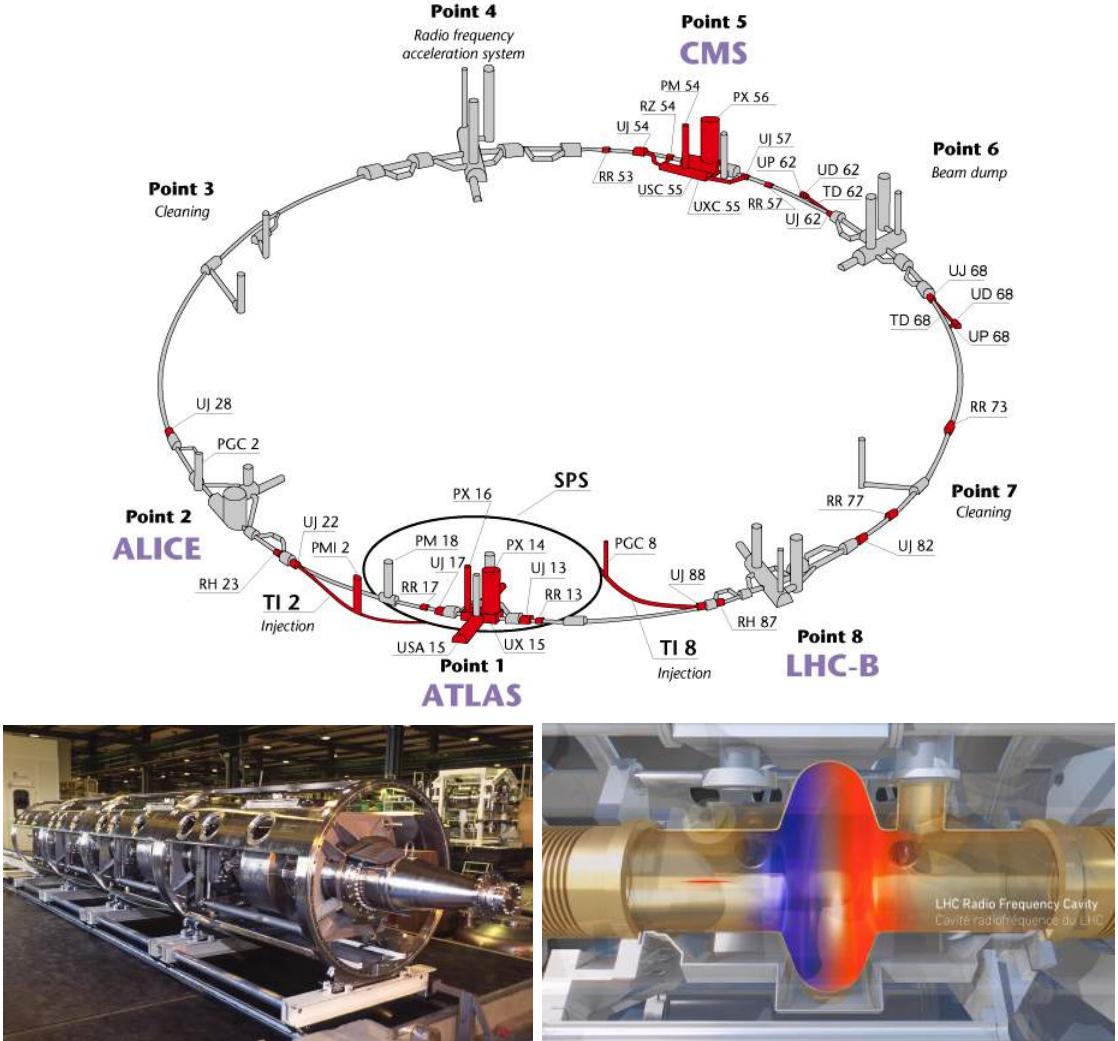


**Figure 2.3:** Left: drawing of the LINAC2 accelerating system at CERN. Electric fields generated by radio frequency (RF) create acceleration and deceleration zones inside the cavity; deceleration zones are blocked by drift tubes where quadrupole magnets focus the proton beam. Right: picture of a real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

1140 Proton bunches coming from the RFQ go to the linear accelerator 2 (LINAC2)  
 1141 where they are accelerated to reach 50 MeV energy. In the LINAC2 stage, acceleration  
 1142 is performed using electric fields generated by radio frequency which create zones  
 1143 of acceleration and deceleration as shown in Figure 2.3. In the deceleration zones,  
 1144 the electric field is blocked using drift tubes where protons are free to drift while  
 1145 quadrupole magnets focus the beam.

1146 The beam coming from LINAC2 is injected into the proton synchrotron booster  
 1147 (PSB) to reach 1.4 GeV in energy. The next acceleration is provided at the proton  
 1148 synchrotron (PS) up to 26 GeV, followed by the injection into the super proton  
 1149 synchrotron (SPS) where protons are accelerated to 450 GeV. Finally, protons are  
 1150 injected into the LHC where they are accelerated to the target energy of 6.5 TeV.

1151 PSB, PS, SPS and LHC accelerate protons using the same RF acceleration tech-  
 1152 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]

1153        The LHC has a system of 16 RF cavities located in the so-called point 4, as  
 1154        shown in Figure 2.4 top, tuned at a frequency of 400 MHz. The bottom side of  
 1155        Figure 2.4 shows a picture of a RF module composed of 4 RF cavities working in a  
 1156        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.

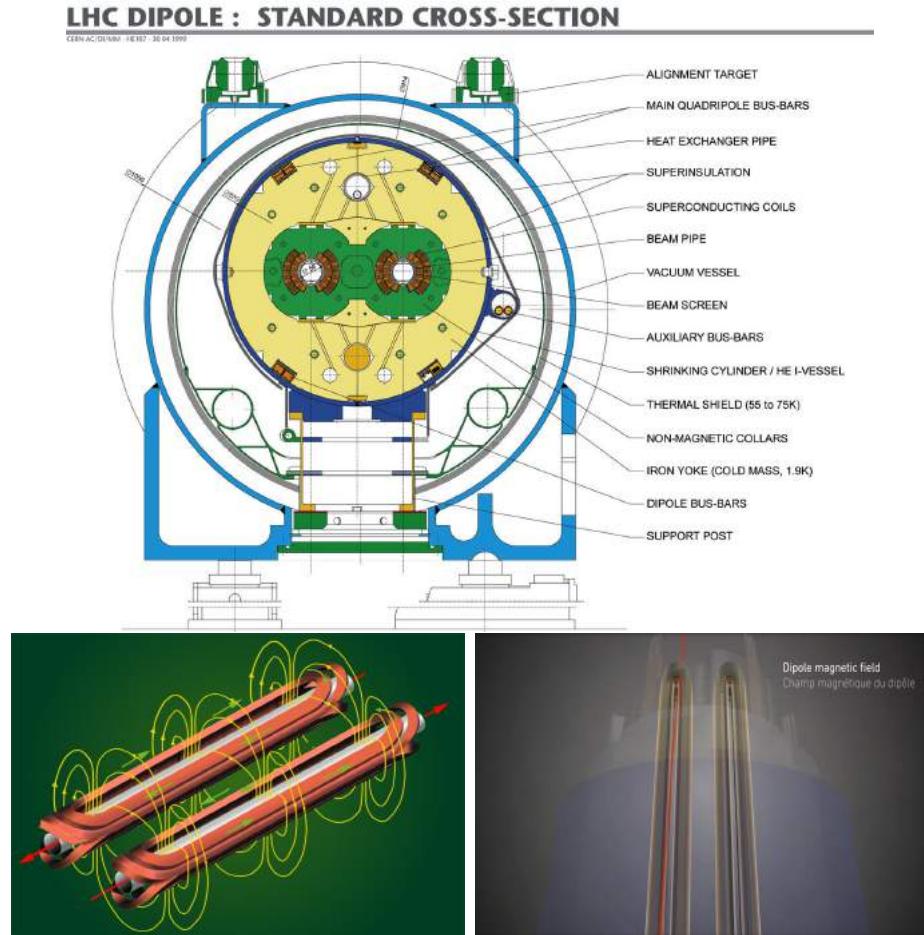
While protons are accelerated in one section of the LHC ring, where the RF cavities are located, in the rest of their path they have to be kept in the curved trajectory defined by the LHC ring. Technically, LHC is not a perfect circle; RF, injection, beam dumping, beam cleaning and sections before and 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].

1180 magnetic field generated by the dipole magnets is shown on the bottom left side of  
 1181 Figure 2.5. The bending effect of the magnetic field on the proton beam is shown on  
 1182 the bottom right side of Figure 2.5. Note that the dipole magnets are not curved;  
 1183 the arc section of the LHC ring is composed of straight dipole magnets of about 15  
 1184 m. In total there are 1232 dipole magnets along the LHC ring.

1185 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

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

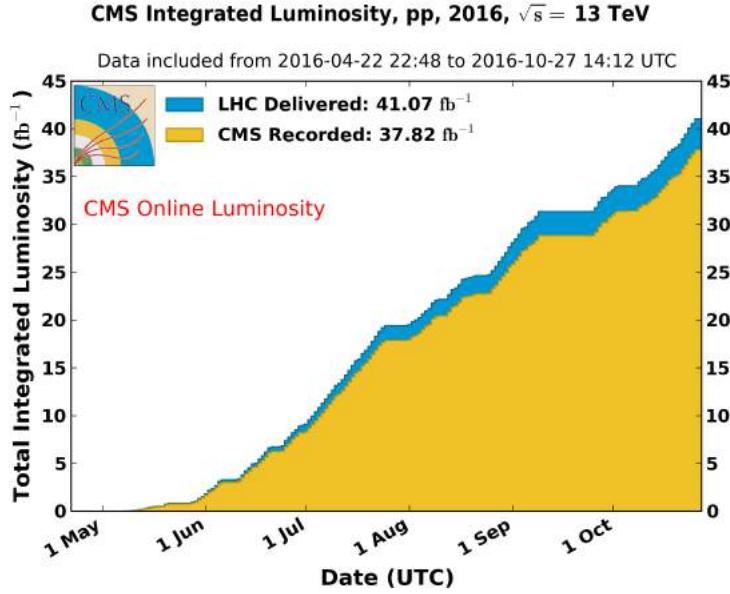
$$n = 2808$$

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

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

1201

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



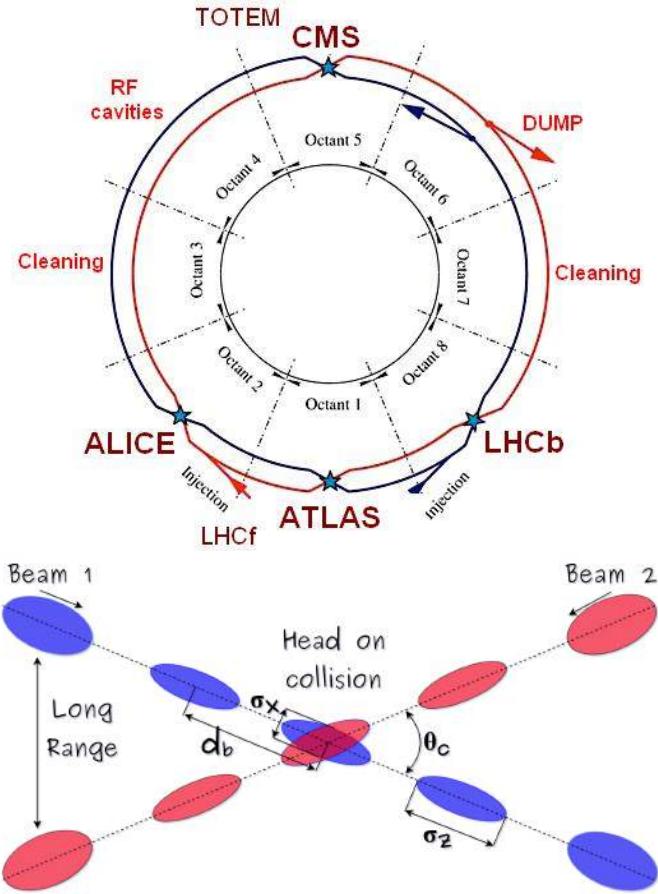
**Figure 2.6:** Integrated luminosity delivered by LHC and recorded by CMS during 2016. The difference between the delivered and the recorded luminosity is due to fails and issues occurred during the data taking in the CMS experiment [71].

1202        Luminosity is a fundamental aspect of LHC given that the bigger luminosity the  
1203        bigger number of collisions, which means that for processes with a very small cross  
1204        section the number of expected occurrences is increased and so the chances of being  
1205        detected. The integrated luminosity, collected by the CMS experiment during 2016  
1206        is shown in Figure 2.6; the data analyzed in this thesis corresponds to an integrated  
1207        luminosity of  $35.9 \text{ fb}^{-1}$  at a center of mass-energy  $\sqrt{s} = 13 \text{ TeV}$ .

1208        One way to increase  $L$  is increasing the number of bunches in the beam. Cur-  
1209        rently, the separation between two consecutive bunches in the beam is 7.5 m which  
1210        corresponds to a time separation of 25 ns. In the full LHC ring the allowed number  
1211        of bunches is  $n = 27\text{km}/7.5\text{m} = 3600$ ; however, there are some gaps in the bunch pat-  
1212        tern intended for preparing the dumping and injection of the beam, thus, the proton  
1213        beams are composed of 2808 bunches.

1214        Once the proton beams reach the desired energy, they are brought to cross each

1215 other producing  $pp$  collisions. The bunch crossing happens in precise places where  
 1216 the four LHC experiments are located, as seen in the top of Figure 2.7. In 2008  $pp$   
 1217 collisions of  $\sqrt{s} = 7$  TeV were performed; the energy was increased to 8 TeV in 2012  
 1218 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].

1219 The CMS and ATLAS experiments are multi-purpose experiments, hence, they  
 1220 are enabled to explore physics in any of the LHC collision modes. LHCb experiment  
 1221 is optimized to explore bottom quark physics, while ALICE is optimized for heavy

1222 ion collisions searches; TOTEM and LHCf are dedicated to forward physics studies;  
 1223 MoEDAL (not indicated in the Figure) is intended for monopole or massive pseudo  
 1224 stable particles searches.

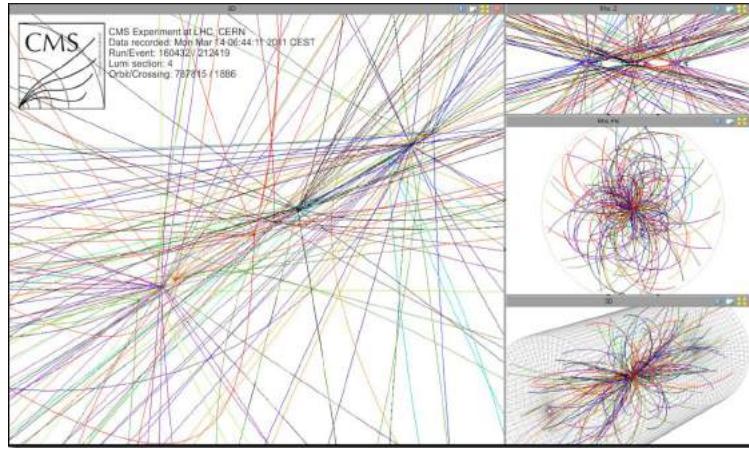
1225 At the IP there are two interesting details that need to be addressed. The first  
 1226 one is that the bunch crossing does not occur head-on but at a small crossing angle  $\theta_c$   
 1227 (280  $\mu$ rad in CMS and ATLAS) as shown in the bottom side of Figure 2.7, affecting  
 1228 the overlapping between bunches; the consequence is a reduction of about 17% in  
 1229 the luminosity (represented by a factor not included in eqn. 2.2). The second one  
 1230 is the occurrence of multiple  $pp$  collisions in the same bunch crossing; this effect is  
 1231 called *pileup* (PU). A fairly simple estimation of the PU follows from estimating the  
 1232 probability of collision between two protons, one from each of the bunches in the  
 1233 course of collision; it depends roughly on the ratio of proton size and the cross section  
 1234 of the bunch in the IP, i.e.,

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

1235 however, there are  $N = 1.15 \times 10^{11}$  protons in a bunch, thus the estimated number of  
 1236 collisions in a bunch crossing is

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

1237 about 20 of which are inelastic. A multiple  $pp$  collision event in a bunch crossing at  
 1238 CMS is shown in Figure 2.8.

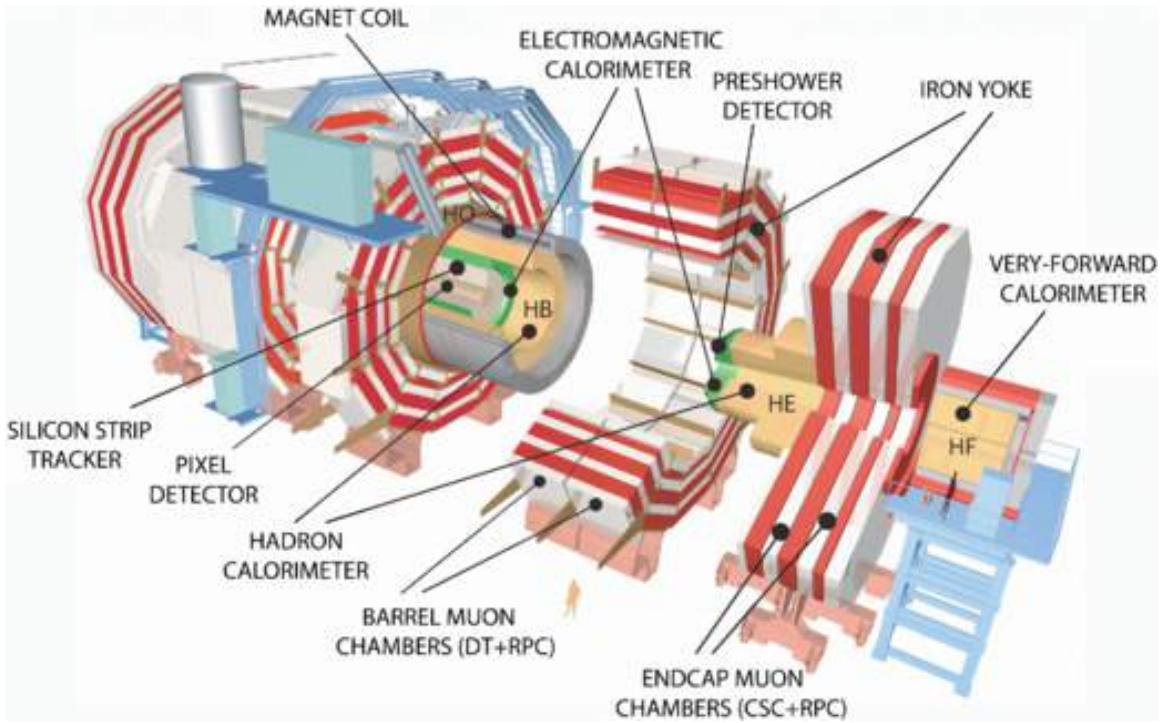


**Figure 2.8:** Multiple  $pp$  collision bunch crossing at CMS. [73].

## 1239    2.3 The CMS experiment

1240 CMS is a general-purpose detector designed to conduct research in a wide range  
 1241 of physics from the standard model to new physics like extra dimensions and dark  
 1242 matter. Located at Point 5 in the LHC layout as shown in Figure 2.4, CMS is  
 1243 composed of several detection systems distributed in a cylindrical structure; in total,  
 1244 CMS weights about 12500 tons in a very compact 21.6 m long and 14.6 m diameter  
 1245 cylinder. It was built in 15 separate sections at the ground level and lowered to the  
 1246 cavern individually to be assembled. A complete and detailed description of the CMS  
 1247 detector and its components is given in Reference [74] on which this section is based.  
 1248 Figure 2.9 shows the layout of the CMS detector. The detection system is composed  
 1249 of (from the innermost to the outermost)

- 1250        • Pixel detector.
- 1251        • Silicon strip tracker.
- 1252        • Preshower detector.
- 1253        • 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].

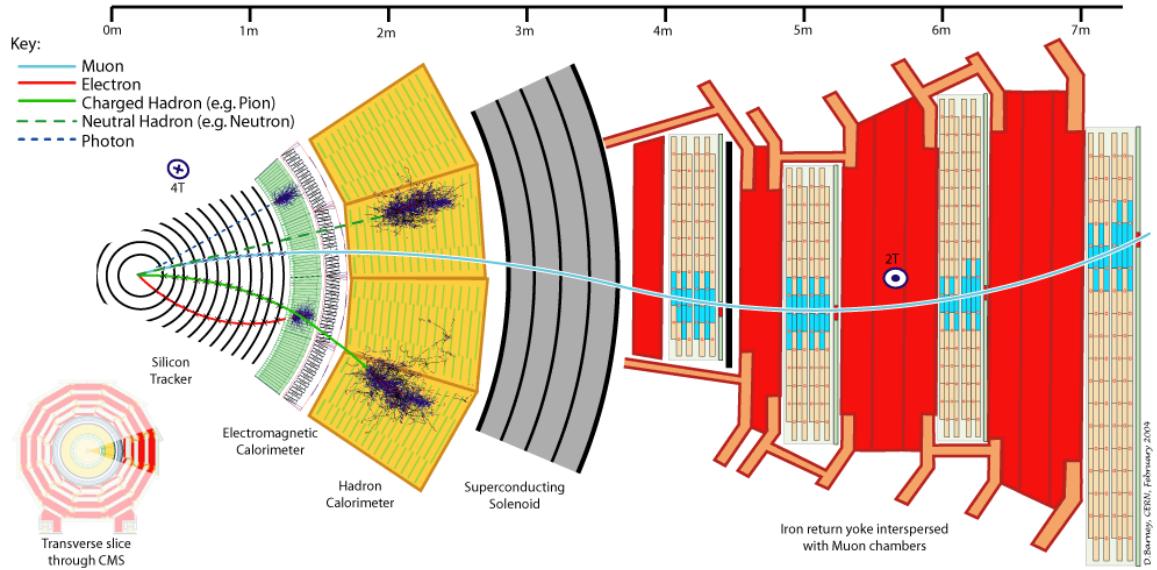
1254        • Hadronic calorimeter.

1255        • Muon chambers (barrel and endcap)

1256        The central region of the detector is commonly referred as the barrel section while  
 1257        the endcaps are referred as the forward sections of the detector; thus, each subdetector  
 1258        is composed of a barrel section and a forward section.

1259        When a  $pp$  collision happens inside the CMS detector, many different particles are  
 1260        produced, but only some of them live long enough to be detected; they are electrons,  
 1261        photons, pions, kaons, protons, neutrons and muons; neutrinos are not detected by  
 1262        the CMS detector. Thus, the CMS detector was designed to detect those particles and  
 1263        measure their properties. Figure 2.10 shows a transverse slice of the CMS detector.  
 1264        The silicon tracker (pixel detector + strip tracker) is capable to register the track of

1265 the charged particles traversing it, while calorimeters (electromagnetic and hadronic)  
 1266 measure the energy of the particles that are absorbed by their materials. Considering  
 1267 the detectable particles, mentioned above, emerging from the IP, a basic description  
 1268 of the detection process is as follows.



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

1269 A muon emerging from the IP, will create a track on the silicon tracker and on  
 1270 the muon chambers. The design of the CMS detector is driven by the requirements  
 1271 on the identification, momentum resolution and unambiguous charge determination  
 1272 of the muons; therefore, a large bending power is provided by the solenoid magnet  
 1273 made of superconducting cable capable of generating a 3.8 T magnetic field. The  
 1274 muon track is bent twice since the magnetic field inside the solenoid is directed along  
 1275 the  $z$ -direction but outside its direction is reversed. Muons interact very weakly with  
 1276 the calorimeters, therefore, it is not absorbed but escape away from the detector.

1277 An electron emerging from the IP will create a track along the tracker which will  
 1278 be bent due to the presence of the magnetic field, later, it will be absorbed in the  
 1279 electromagnetic calorimeter where its energy is measured.

1280        A photon will not leave a track because it is neutral, but it will be absorbed in  
 1281        the electromagnetic calorimeter.

1282        A neutral hadron, like the neutron, will not leave a track either but it will lose a  
 1283        small amount of its energy during its passage through the electromagnetic calorimeter  
 1284        and then it will be absorbed in the hadron calorimeter depositing the rest of its energy.

1285        A charged hadron, like the proton or  $\pi^\pm$ , will leave a curved track on the silicon  
 1286        tracker, some of its energy in the electromagnetic calorimeter and finally will be  
 1287        absorbed in the hadronic calorimeter.

1288        A more detailed description of each detection system will be presented in the  
 1289        following sections.

### 1290        2.3.1 CMS coordinate system

1291        The coordinate system used by CMS is centered on the geometrical center of the  
 1292        detector which is the nominal IP as shown in Figure 2.11<sup>1</sup>. The  $z$ -axis is parallel  
 1293        to the beam direction, while the  $Y$ -axis pointing vertically upward, and the  $X$ -axis  
 1294        pointing radially inward toward the center of the LHC.

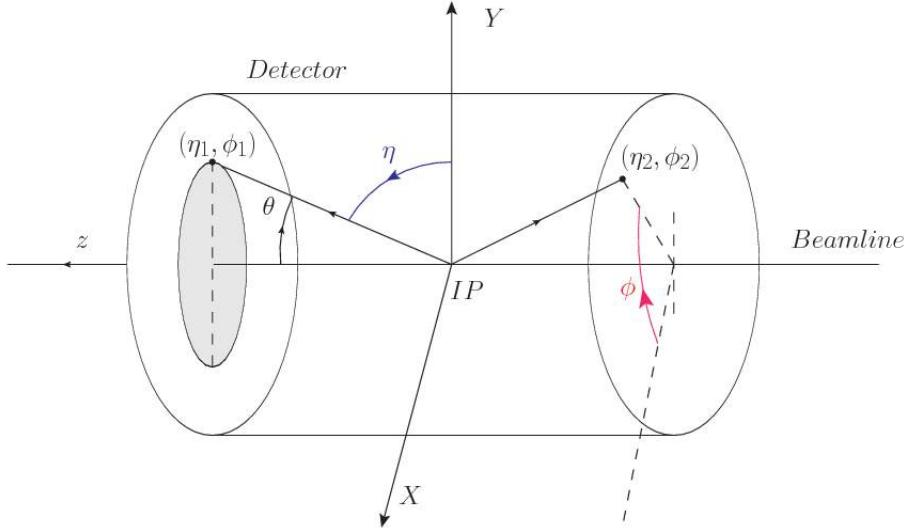
1295        In addition to the common cartesian and cylindrical coordinate systems, two co-  
 1296        ordinates are of particular utility in particle physics: rapidity ( $y$ ) and pseudorapidity  
 1297        ( $\eta$ ), defined in connection to the polar angle  $\theta$ , energy and longitudinal momentum  
 1298        component (momentum along the  $z$ -axis) according to

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

1299        Rapidity is related to the angle between the  $XY$ -plane and the direction in which  
 1300        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.

1301 between the rapidities of two particles is invariant with respect to Lorentz boosts  
 1302 along the  $z$ -axis, hence, data analysis becomes more simple when based on rapid-  
 1303 ity; however, it is not simple to measure the rapidity of highly relativistic particles,  
 1304 as those produced after  $pp$  collisions. Under the highly relativistic motion approxi-  
 1305 mation,  $y$  can be rewritten in terms of the polar angle, concluding that rapidity is  
 1306 approximately equal to the pseudorapidity defined above, i.e.,  $y \approx \eta$ . Note that  $\eta$   
 1307 is easier to measure than  $y$  given the direct relationship between the former and the  
 1308 polar angle.

1309       The angular distance between two objects in the detector ( $\Delta R$ ) is commonly used  
 1310 to judge the isolation of those object; it is defined in terms of their coordinates  $(\eta_1, \phi_1)$ ,  
 1311  $(\eta_2, \phi_2)$  as

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

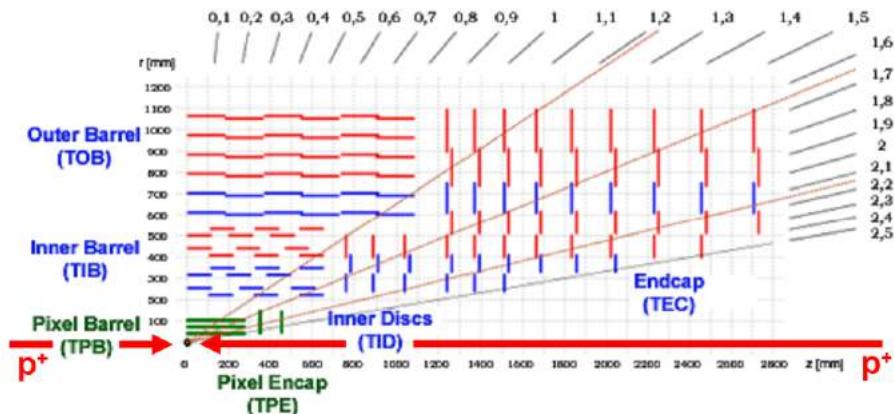
### 1312 2.3.2 Tracking system

1313 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  
 1314 precise reconstruction of the primary and secondary origins of the tracks (*vertices*) is  
 1315 expected in an environment where, each 25 ns, the bunch crossing produces about 20  
 1316 inelastic collisions and about 1000 particles.  
 1317

1318 Physics requirements guiding the tracking system performance include the precise characterization of events involving gauge bosons, W and Z, and their leptonic  
 1319 decays for which an efficient isolated lepton and photon reconstruction is of capital  
 1320 importance, given that isolation is required to suppress background events to a level  
 1321 that allows observations of interesting processes like Higgs boson decays or beyond  
 1322 SM events.

1324 The ability to identify and reconstruct  $b$ -jets and B-hadrons within these jets is also  
 1325 a fundamental requirement, achieved through the ability to reconstruct accurately  
 1326 displaced vertices, given that  $b$ -jets are part of the signature of top quark physics, like  
 1327 the one treated in this thesis.

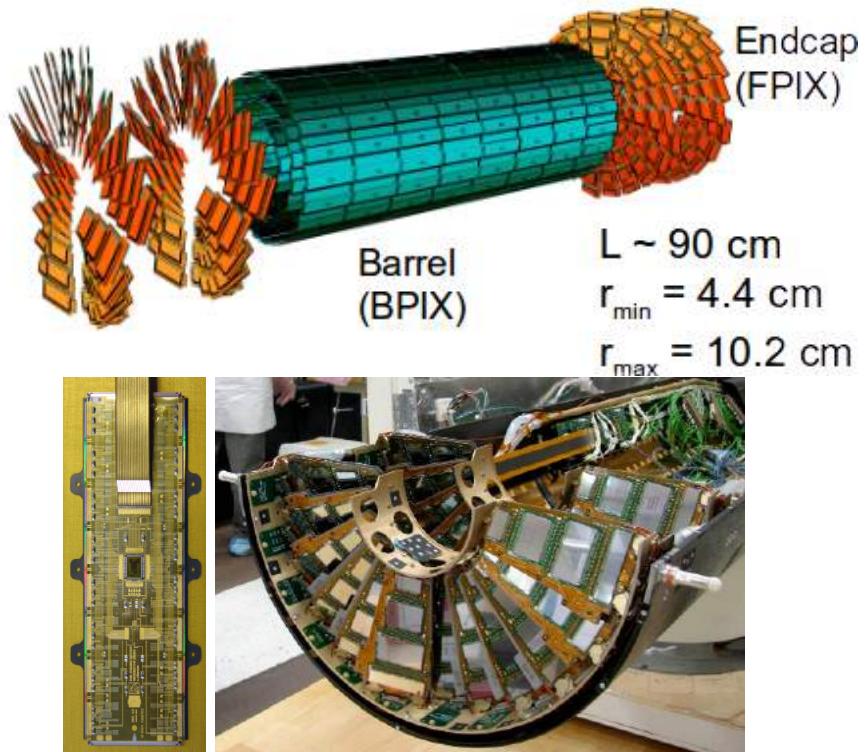
1328 An schematic view of the CMS tracking system is shown in Figure 2.12



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

1329 In order to satisfy these performance requirements, the tracking system uses two  
 1330 different detector subsystems arranged in concentric cylindrical volumes, the pixel  
 1331 detector and the silicon strip tracker; the pixel detector is located in the high particle  
 1332 density region ( $r < 20\text{cm}$ ) while the silicon strip tracker is located in the medium and  
 1333 lower particle density regions  $20\text{cm} < r < 116\text{cm}$ .

1334 **Pixel detector**



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

1335 The pixel detector was replaced during the 2016-2017 extended year-end technical  
 1336 stop, due to the increasingly challenging operating conditions like the higher particle  
 1337 flux and more radiation harsh environment, among others. The new one is responding  
 1338 as expected, reinforcing its crucial role in the successful way to fulfill the new LHC

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

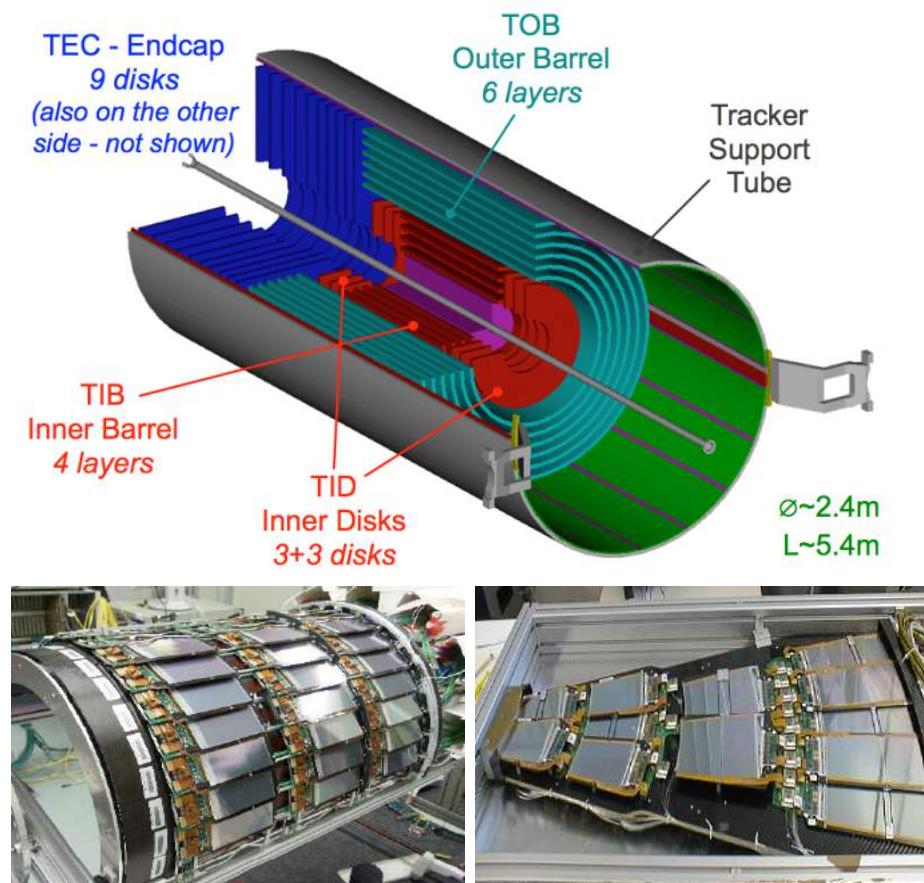
The pixel detector was composed of 1440 silicon pixel detector modules organized in three-barrel layers in the central region (BPix) and two disks in the forward region (FPix) as shown in the top side of Figure 2.13; it was designed to record efficiently and with high precision, up to  $20\mu\text{m}$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

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

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

1365 blades in the turbine-like layout as shown in Figure 2.13 bottom left.

### 1366 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].

1367 The silicon strip tracker (SST) is the second stage in the CMS tracking system.

1368 The top side of Figure 2.14 shows a schematic of the SST. The inner tracker region is

1369 composed of the tracker inner barrel (TIB) and the tracker inner disks (TID) covering

1370 the region  $r < 55$  cm and  $|z| < 118$  cm. The TIB is composed of 4 layers while the TID

1371 is composed of 3 disks at each end. The silicon sensors in the inner tracker are 320  
 1372  $\mu\text{m}$  thick, providing a resolution of about 13-38  $\mu\text{m}$  in the  $r\phi$  position measurement.

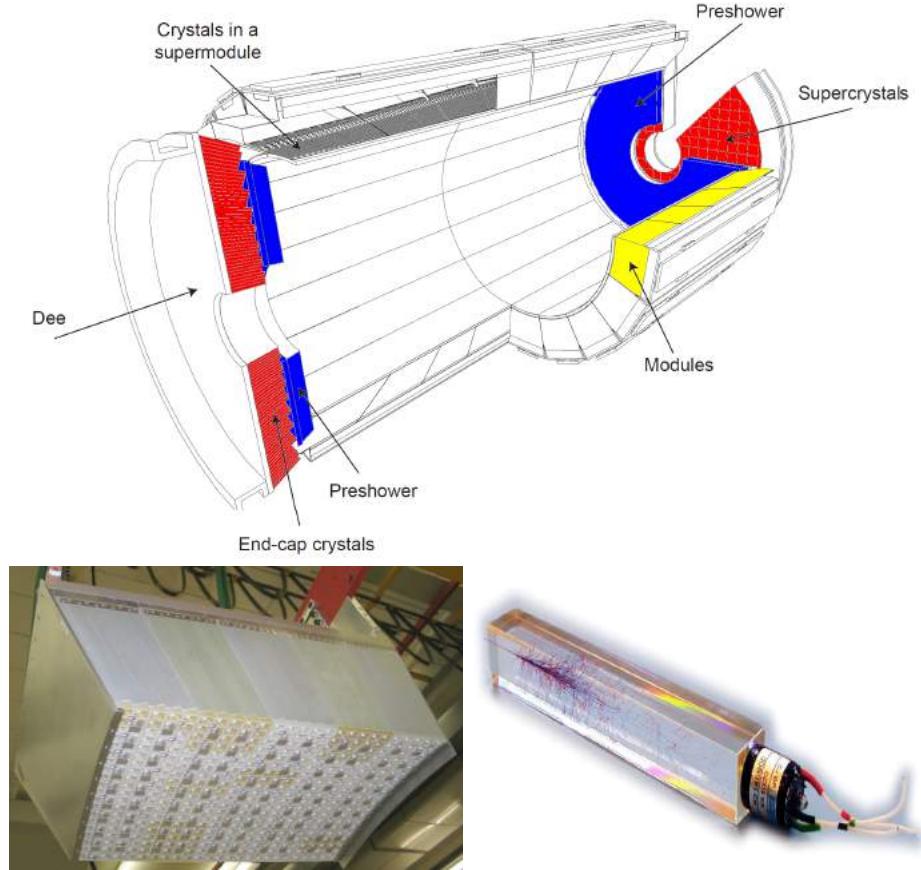
1373       The modules indicated in blue in the schematic view of Figure 2.14 are two mod-  
 1374 ules mounted back-to-back and rotated in the plane of the module by a *stereo* angle  
 1375 of 100 mrad; the hits from these two modules, known as *stereo hits*, are combined to  
 1376 provide a measurement of the second coordinate ( $z$  in the barrel and  $r$  on the disks)  
 1377 allowing the reconstruction of hit positions in 3-D.

1378       The outer tracker region is composed of the tracker outer barrel (TOB) and the  
 1379 tracker endcaps (TEC). The six layers of the TOB offer coverage in the region  $r > 55$   
 1380 cm and  $|z| < 118$  cm, while the 9 disks of the TEC cover the region  $124 < |z| < 282$   
 1381 cm. The resolution offered by the outer tracker is about 13-38  $\mu\text{m}$  in the  $r\phi$  position  
 1382 measurement. The inner four TEC disks use silicon sensors 320  $\mu\text{m}$  thick; those in  
 1383 the TOB and the outer three TEC disks use silicon sensors of 500  $\mu\text{m}$  thickness. The  
 1384 silicon strips run parallel to the  $z$ -axis and the distance between strips varies from 80  
 1385  $\mu\text{m}$  in the inner TIB layers to 183  $\mu\text{m}$  in the inner TOB layers; in the endcaps the  
 1386 wedge-shaped sensors with radial strips, whose pitch range between 81  $\mu\text{m}$  at small  
 1387 radii and 205  $\mu\text{m}$  at large radii.

1388       The whole SST has 15148 silicon modules, 9.3 million silicon strips and cover a  
 1389 total active area of about 198  $\text{m}^2$ .

### 1390     **2.3.4 Electromagnetic calorimeter**

1391       The CMS electromagnetic calorimeter (ECAL) is designed to measure the energy of  
 1392 electrons and photons. It is composed of 75848 lead tungstate crystals which have a  
 1393 short radiation length (0.89 cm) and fast response, since 80% of the light is emitted  
 1394 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].

1395 photodetectors given that crystals themselves have a low light yield ( $30\gamma/\text{MeV}$ ). A  
 1396 schematic view of the ECAL is shown in Figure 2.15.

1397 Energy is measured when electrons and photons are absorbed by the crystals  
 1398 which generates an electromagnetic *shower*, as seen in bottom right picture of the  
 1399 Figure 2.15; the shower is seen as a *cluster* of energy which depending on the amount  
 1400 of energy deposited can involve several crystals. The ECAL barrel (EB) covers the  
 1401 region  $|\eta| < 1.479$ , using crystals of depth of 23 cm and  $2.2 \times 2.2 \text{ cm}^2$  transverse  
 1402 section; the ECAL endcap (EE) covers the region  $1.479 < |\eta| < 3.0$  using crystals of  
 1403 depth 22 cm and transverse section of  $2.86 \times 2.86 \text{ cm}^2$ ; the photodetectors used are

1404 vacuum phototriodes (VPTs). Each EE is divided in two structures called *Dees*.

1405       The preshower detector (ES) is installed in front of the EE and covers the region  
 1406       $1.653 < |\eta| < 2.6$ . The ES provides a precise measurement of the position of electro-  
 1407      magnetic showers, which allows to distinguish electrons and photon signals from  $\pi^0$   
 1408      decay signals. The ES is composed of a layer of lead radiators followed by a layer of  
 1409      silicon strip sensors. The lead radiators initiate electromagnetic showers when reached  
 1410      by photons and electrons, then, the strip sensors measure the deposited energy and  
 1411      the transverse shower profiles. The full ES thickness is 20 cm.

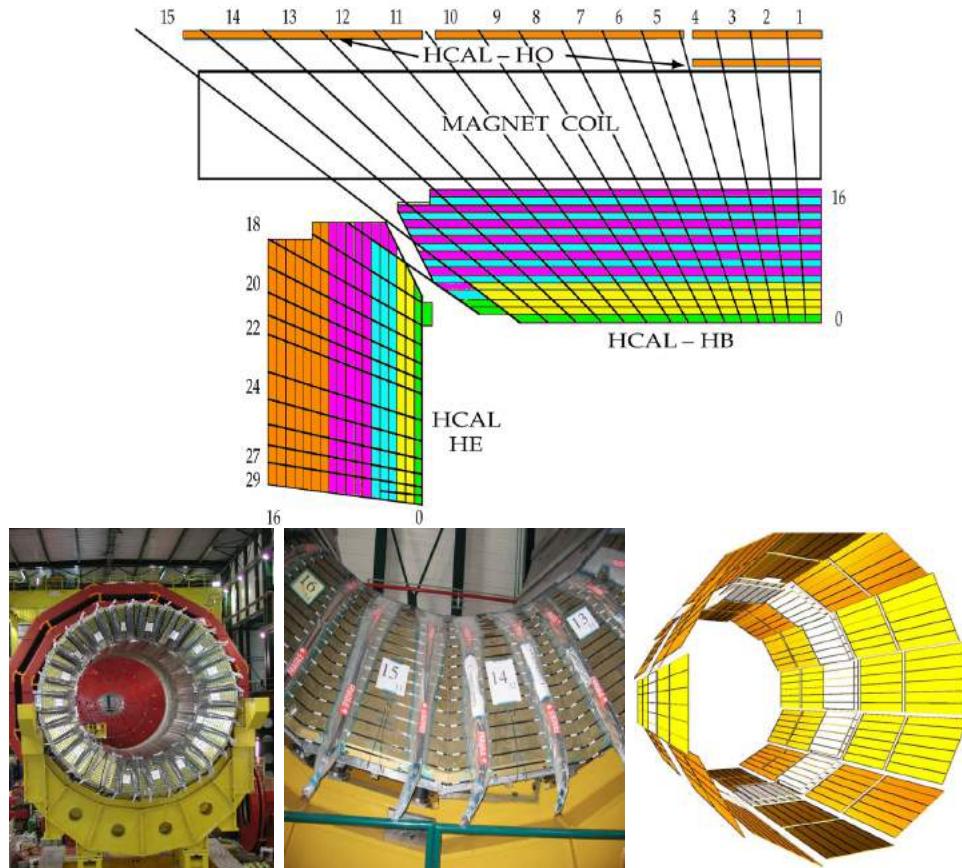
### 1412     **2.3.5 Hadronic calorimeter**

1413   Hadrons are not absorbed by the ECAL<sup>2</sup> but by the hadron calorimeter (HCAL),  
 1414   which is made of a combination of alternating brass absorber layers and silicon photo-  
 1415   multiplier(SiPM) layers; therefore, particles passing through the scintillator material  
 1416   produce showers, as in the ECAL, as a result of the inelastic scattering of the hadrons  
 1417   with the detector material. Since the particles are not absorbed in the scintillator,  
 1418   their energy is sampled; therefore the total energy is not measured but estimated from  
 1419   the energy clusters, which reduces the resolution of the detector. Brass was chosen  
 1420   as the absorber material due to its short interaction length ( $\lambda_I = 16.42\text{cm}$ ) and its  
 1421   non-magnetivity. Figure 2.16 shows a schematic view of the CMS HCAL.

1422       The HCAL is divided into four sections; the Hadron Barrel (HB), the Hadron  
 1423       Outer (HO), the Hadron Endcap (HE) and the Hadron Forward (HF) sections. The  
 1424       HB covers the region  $0 < |\eta| < 1.4$ , while the HE covers the region  $1.3 < |\eta| < 3.0$ .  
 1425       The HF, made of quartz fiber scintillator and steel as absorption material, covers the  
 1426       forward region  $3.0 < |\eta| < 5.2$ . Both the HB and HF are located inside the solenoid.  
 1427       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.

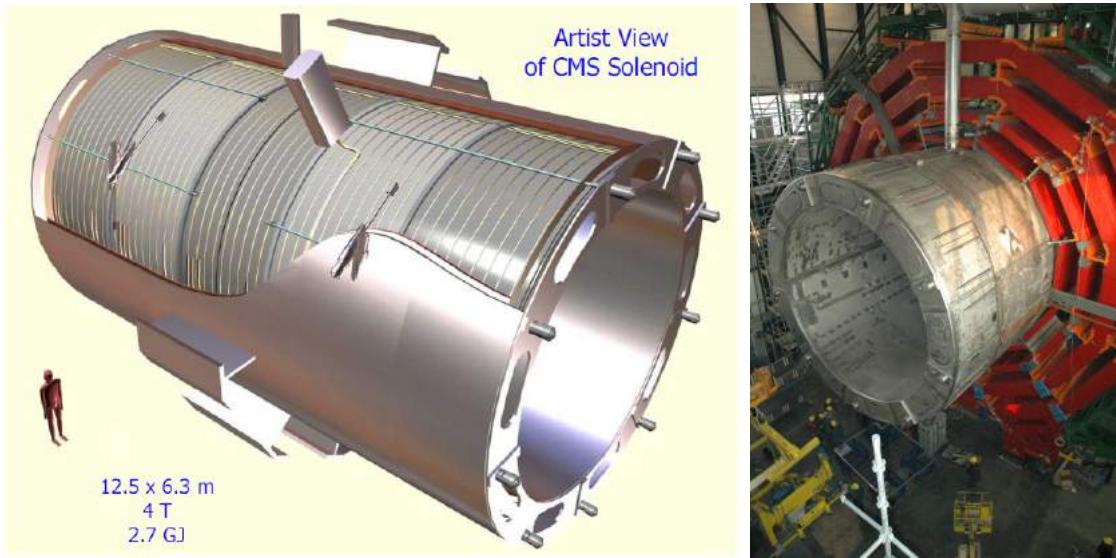


**Figure 2.16:** Top: CMS HCAL schematic view, the colors indicate the layers that are grouped into the same readout channels. Bottom: picture of a section of the HB; the absorber material is the golden region and scintillators are placed in between the absorber material (left and center). Schematic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

1428 purpose of measure the energy tails of particles passing through the HB and the  
 1429 magnet (see Figure 2.16 top and bottom right).

### 1430 **2.3.6 Superconducting solenoid magnet**

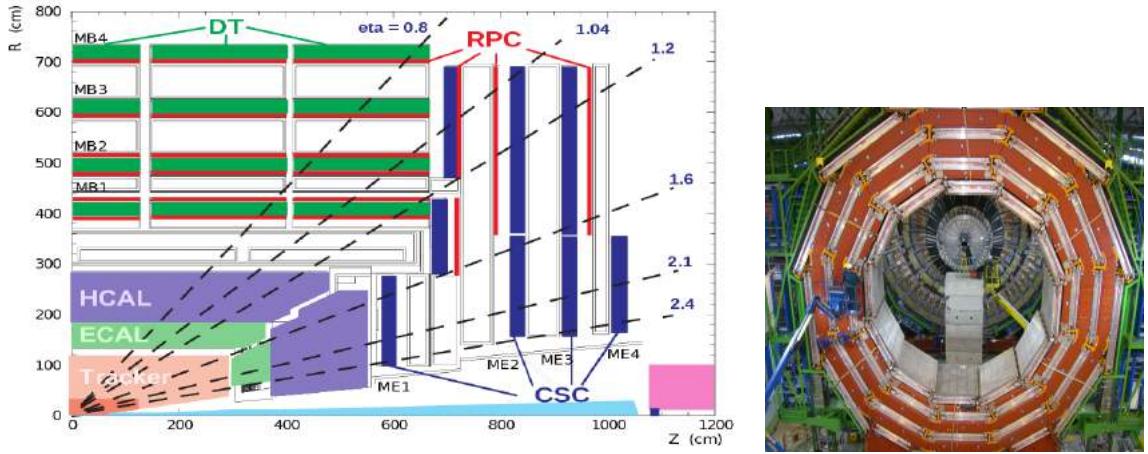
1431 The superconducting magnet installed in the CMS detector is designed to provide  
 1432 an intense and highly uniform magnetic field in the central part of the detector.  
 1433 In fact, the tracking system takes advantage of the bending power of the magnetic  
 1434 field to measure with precision 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].

1435 unambiguous determination of the sign for high momentum muons was a driving  
 1436 principle during the design of the magnet. The magnet has a diameter of 6.3 m, a  
 1437 length of 12.5 m and a cold mass of 220 t; the generated magnetic field reaches a  
 1438 strength of 3.8T. Since it is made of Ni-Tb superconducting cable it has to operate at  
 1439 a temperature of 4.7 K by using a helium cryogenic system; the current circulating in  
 1440 the cables reaches 18800 A under normal running conditions. The left side of Figure  
 1441 2.17 shows an artistic view of the CMS magnet, while the right side shows a transverse  
 1442 view of the cold mass where the winding structure is visible.

1443 The yoke (see Figure 2.17), composed of 5 barrel wheels and 6 endcap disks made  
 1444 of iron, serves not only as the media for magnetic flux return but also provides housing  
 1445 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].

### 1446 2.3.7 Muon system

1447 Muons are the only charged particles able to pass through all the CMS detector due  
 1448 to their low ionization energy loss; thus, muons can be separated easily from the  
 1449 high amount of particles produced in a  $pp$  collision. Also, muons are expected to be  
 1450 produced in the decay of several new particles; therefore, good detection of muons  
 1451 was one of the leading principles when designing the CMS detector.

1452 The CMS muon detection system (muon spectrometer) is embedded in the return  
 1453 yoke as seen in Figure 2.18. It is composed of three different detector types, the drift  
 1454 tube chambers (DT), cathode strip chambers (CSC), and resistive plate chambers  
 1455 (RPC); DT are located in the central region  $\eta < 1.2$  arranged in four layers of drift  
 1456 chambers filled with an Ar/CO<sub>2</sub> gas mixture.

1457 The muon endcaps are made of CSCs covering the region  $\eta < 2.4$  and filled with  
 1458 a mixture of Ar/CO<sub>2</sub>/CF<sub>4</sub>. The reason behind using a different detector type lies on  
 1459 the different conditions in the forward region like the higher muon rate and higher  
 1460 residual magnetic field compared to the central region.

1461 The third type of detector used in the muon system is a set of four disks of RPCs

1462 working in avalanche mode. The RPCs provide good spatial and time resolutions. The  
 1463 track of high- $p_T$  muon candidates is built combining information from the tracking  
 1464 system and the signal from up to six RPCs and four DT chambers.

1465 The muon tracks are reconstructed from the hits in the several layers of the muon  
 1466 system.

### 1467 **2.3.8 CMS trigger system**

1468 CMS expects  $pp$  collisions every 25 ns, i.e., an interaction rate of 40 MHz for which  
 1469 it is not possible to store the recorded data in full. In order to handle this high event  
 1470 rate data, an online event selection, known as triggering, is performed; triggering  
 1471 reduces the event rate to 100 Hz for storage and further offline analysis.

1472 The trigger system starts with a reduction of the event rate to 100 kHz in the  
 1473 so-called *the level 1 trigger* (L1). L1 is based on dedicated programmable hardware  
 1474 like Field Programmable Gate Arrays (FPGAs) and Application Specific Integrated  
 1475 Circuits (ASICs), partly located in the detector itself; another portion is located in  
 1476 the CMS underground cavern. Hit pattern information from the muon chambers  
 1477 and the energy deposits in the calorimeter are used to decide if an event is accepted  
 1478 or rejected, according to selection requirements previously defined, which reflect the  
 1479 interesting physics processes. Figure 2.19 shows the L1 trigger architecture.

1480 The second stage in the trigger system is called *the high-level trigger* (HLT); events  
 1481 accepted by L1 are passed to HLT in order to make an initial reconstruction of them.  
 1482 HLT is software based and runs on a dedicated server farm, using selection algorithms  
 1483 and high-level object definitions; the event rate at HLT is reduced to 100 Hz. The  
 1484 first HLT stage takes information from the muon detectors and the calorimeters to  
 1485 make the initial object reconstruction; in the next HLT stage, information from the

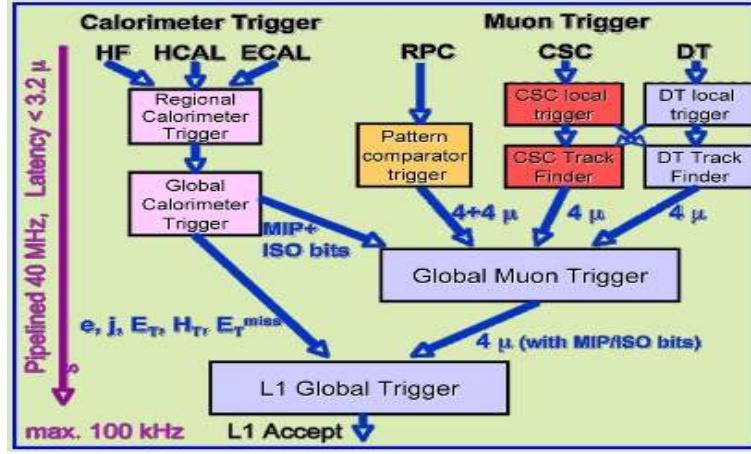


Figure 2.19: CMS Level-1 trigger architecture [86].

pixel and strip detectors is used to do first fast tracking and then full tracking online.

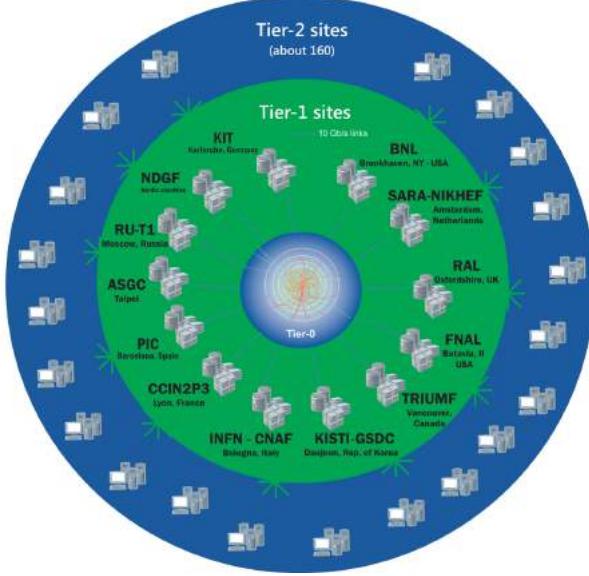
This initial object reconstruction is used in further steps of the trigger system.

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].

1502 that distributed environment. WLCG is a tiered structure connecting computing  
 1503 centers around the world, which provides the necessary storage and computing facil-  
 1504 ities. The primary computing centers of the WLCG are located at the CERN and  
 1505 the Wigner datacenter in Budapest and are known as Tier-0 as shown in Figure 2.20.  
 1506 The main responsibilities for each tier level are [87]

- 1507     • **Tier-0:** initial reconstruction of recorded events and storage of the resulting  
       1508 datasets, the distribution of raw data to the Tier-1 centers.
- 1509     • **Tier-1:** provide storage capacity, support for the Grid, safe-keeping of a pro-  
       1510 portional share of raw and reconstructed data, large-scale reprocessing and safe-  
       1511 keeping of corresponding output, generation of simulated events, distribution  
       1512 of data to Tier 2s, safe-keeping of a share of simulated data produced at these  
       1513 Tier 2s.
- 1514     • **Tier-2:** store sufficient data and provide adequate computing power for spe-

1515       cific analysis tasks and proportional share of simulated event production and  
1516       reconstruction.

1517       Aside from the general computing strategy to manage the huge amount of data  
1518       produced by experiments, CMS uses a software framework to perform a variety of  
1519       processing, selection and analysis tasks. The central concept of the CMS data model  
1520       referred to as *event data model* (EDM) is the *Event*; therefore, an event is the unit  
1521       that contains the information from a single bunch crossing, any data derived from  
1522       that information like the reconstructed objects, and the details of the derivation.

1523       Events are passed as the input to the *physics modules* that obtain information  
1524       from them and create new information; for instance, *event data producers* add new  
1525       data into the events, *analyzers* produce an information summary from an event set,  
1526       *filters* perform selection and triggering.

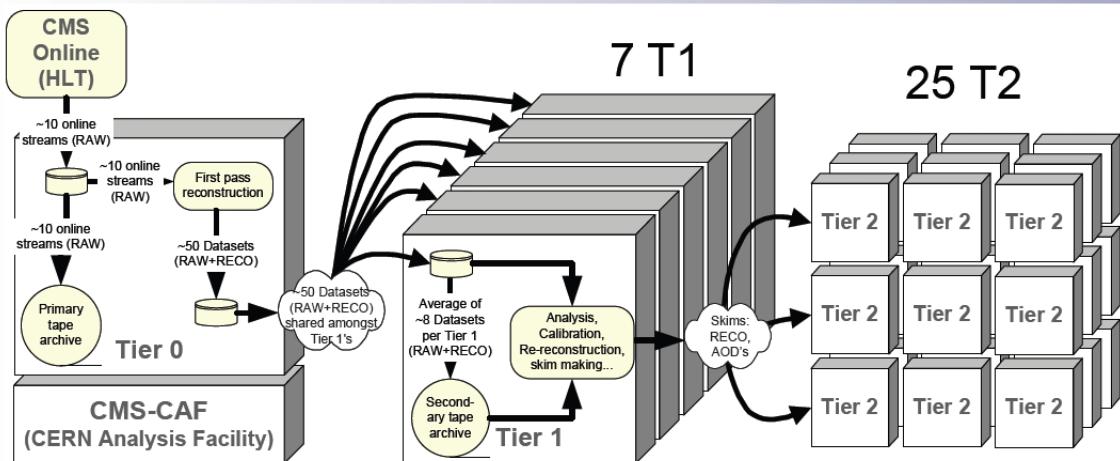
1527       CMS uses several event formats with different levels of detail and precision

1528       • **Raw format:** events in this format contain the full recorded information from  
1529       the detector as well as trigger decision and other metadata. An extended version  
1530       of raw data is used to store information from the CMS Monte Carlo simulation  
1531       tools (see Chapter 3). Raw data are stored permanently, occupying about  
1532       2MB/event

1533       • **RECO format:** events in this format correspond to raw data that have been  
1534       submitted to reconstruction algorithms like primary and secondary vertex re-  
1535       construction, particle ID, and track finding. RECO events contain physics ob-  
1536       jects and all the information used to reconstruct them; average size is about 0.5  
1537       MB/event.

- 1538     • **AOD format:** Analysis Object Data (AOD) is the data format used in the  
 1539        physics analyses given that it contains the parameters describing the high-level  
 1540        physics objects in addition to enough information to allow a kinematic refitting if  
 1541        needed. AOD events are filtered versions of the RECO events to which skimming  
 1542        or other filtering have been applied, hence AOD events are subsets of RECO  
 1543        events. Requires about 100 kB/event.
- 1544     • **Non-event data** are data needed to interpret and reconstruct events. Some  
 1545        of the non-event data used by CMS contains information about the detector  
 1546        contraction and condition data like calibrations, alignment, and detector status.

1547     Figure 2.21 shows the data flow scheme between CMS detector and tiers.



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

1548     The whole collection of software built as a framework is referred to as *CMSSW*. This  
 1549        framework provides the services needed by the simulation, calibration and alignment,  
 1550        and reconstruction modules that process event data, so that physicists can perform  
 1551        analysis. The CMSSW event processing model is composed of one executable, called  
 1552        cmsRun, and several plug-in modules which contains all the tools (calibration, recon-

1553 struction algorithms) needed to process an event. The same executable is used for  
1554 both detector data and Monte Carlo simulations [88].

1555 **Chapter 3**

1556 **Event generation, simulation and  
1557 reconstruction**

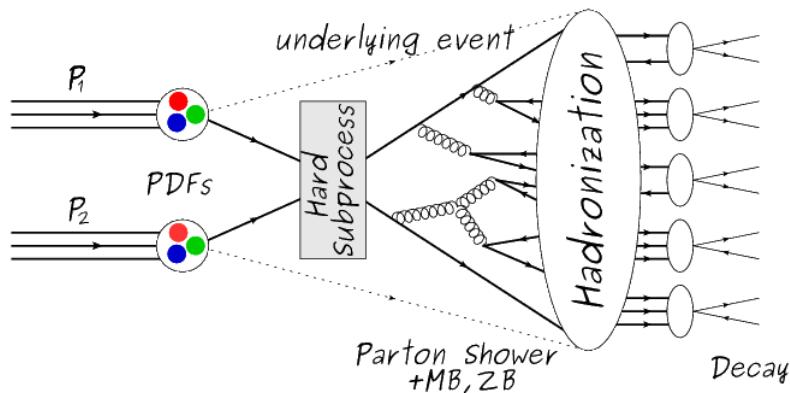
1558 The process of analyzing data recorded by the CMS experiment involves several stages  
1559 where the data are processed in order to interpret the information provided by all  
1560 the detection systems; in those stages, the particles produced after the  $pp$  collision  
1561 are identified by reconstructing their trajectories and measuring their features. In  
1562 addition, the SM provides a set of predictions that have to be compared with the  
1563 experimental results; however, in most of the cases, theoretical predictions are not  
1564 directly comparable to experimental results due to the diverse source of uncertainties  
1565 introduced by the experimental setup and theoretical approximations, among others.

1566 The strategy to face these conditions consists in using statistical methods imple-  
1567 mented in computational algorithms to produce numerical results that can be con-  
1568 trasted with the experimental results. These computational algorithms are commonly  
1569 known as Monte Carlo (MC) methods and, in the case of particle physics, they are  
1570 designed to apply the SM rules and produce predictions about the physical observ-  
1571 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.

1586 Generation starts by taking into account the PDFs of the incoming particles.  
 1587 Event generators offer the option to chose from several PDF sets depending on the  
 1588 particular process under simulation<sup>1</sup>; in the following,  $pp$  collisions will be consid-  
 1589 ered. The *hard subprocess* describes the actual interaction between partons from the  
 1590 incoming protons; it is represented by the matrix element connecting the initial and  
 1591 final states of the interaction. Normally, the matrix element can be written as a  
 1592 sum over Feynman diagrams and consider interferences between terms in the sum-  
 1593 mation. During the generation of the hard subprocess, the production cross section  
 1594 is calculated.

1595 The order to which the cross section is calculated depends on the order of the Feyn-  
 1596 man diagrams involved in the calculation; therefore, radiative corrections are included  
 1597 by considering a higher order Feynman diagrams where QCD radiation dominates.  
 1598 Currently, cross sections calculated to LO do not offer a satisfactory description of the  
 1599 processes, i.e., the results are only reliable for the shape of distributions; therefore,  
 1600 NLO calculations have to be performed with the implication that the computing time  
 1601 needed is highly increased.

1602 The final parton content of the hard subprocess is subjected to the *parton shower*  
 1603 which generates the gluon radiation. Parton shower evolves the partons, i.e., glouns  
 1604 split into quark-antiquark pairs and quarks with enough energy radiate gluons giv-  
 1605 ing rise to further parton multiplication, following the DGLAP (Dokshitzer-Gribov-  
 1606 Lipatov-Altarelli-Parisi) equations. Showering continues until the energy scale is low  
 1607 enough to reach the non-perturbative limit.

1608 In the simulation of LHC processes that involve  $b$  quarks, like the single top quark  
 1609 or Higgs associated production, it is needed to consider that the  $b$  quark is heavier  
 1610 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.

1611 schemes [95]

- 1612     • four-flavor (4F) scheme.  $b$  quarks appear only in the final state because they  
 1613       are heavier than the proton and therefore they can be produced only from the  
 1614       splitting of a gluon into pairs or singly in association with a  $t$  quark in high  
 1615       energy-scale interactions; furthermore, during the simulation, the  $b$ -PDFs are set  
 1616       to zero. Calculations in this scheme are more complicated due to the presence  
 1617       of the second  $b$  quark but the full kinematics is considered already at LO and  
 1618       therefore the accuracy of the description is better.
- 1619     • five-flavor (5F) scheme.  $b$  quarks are considered massless, therefore they can  
 1620       appear in both initial and final states since they can now be part of the proton;  
 1621       thus, during the simulation  $b$ -PDFs are not set to zero. In this scheme, calcula-  
 1622       tions are simpler than in the 4F scheme and possible logarithmic divergences  
 1623       are absorbed by the PDFs through the DGLAP evolution.

1624     In this thesis, the  $tHq$  events are generated using the 4F scheme in order to reduce  
 1625     uncertainties, while the  $tHW$  events are generated using the 5F scheme to eliminate  
 1626     LO interference with  $t\bar{t}H$  process [48].

1627     Partons involved in the  $pp$  collision are the focus of the simulation, however, the  
 1628     rest of the partons inside the incoming protons are also affected because the remnants  
 1629     are colored objects; also, multiple parton interactions can occur. The hadronization  
 1630     of the remnants and multiple parton interactions are known as *underlying event* and  
 1631     it has to be included in the simulation. In addition, multiple  $pp$  collisions in the same  
 1632     bunch crossing (pile-up mentioned in 2.2) occurs, actually in two forms

- 1633     • *in-time PU* which refers to multiple  $pp$  collision in the bunch crossing but that  
 1634       are not considered as primary vertices.

1635       • *Out-of-time PU* which refers to overlapping  $pp$  collisions from consecutive bunch  
 1636       crossings; this can occur due to the time-delays in the detection systems where  
 1637       information from one bunch crossing is assigned to the next or previous one.

1638       While the underlying event effects are included in generation using generator-  
 1639       specific tools, PU effects are added to the generation by overlaying Minimum-bias (MB)  
 1640       and Zero-bias (ZB) events to the generated events. MB events are inelastic events  
 1641       selected by using a loose trigger with as little bias as possible, therefore accepting a  
 1642       large fraction of the overall inelastic event; ZB events correspond to random events  
 1643       recorded by the detector when collisions are likely. MB models in-time PU and ZB  
 1644       models out-of-time PU.

1645       The next step in the generation process is called *hadronization*. Since particles  
 1646       with a net color charge are not allowed to exits isolated, they have to recombine  
 1647       to form bound states. This is precisely the process by which the partons resulting  
 1648       from the parton shower arrange themselves as color singlets to form hadrons. At  
 1649       this step, the energy-scale is low and the strong coupling constant is large, therefore  
 1650       hadronization process is non-perturbative and the evolution of the partons is described  
 1651       using phenomenological models. Most of the baryons and mesons produced in the  
 1652       hadronization are unstable and hence they will decay in the detector.

1653       The last step in the generation process corresponds to the decay of the unstable  
 1654       particles generated during hadronization; it is also simulated in the hadronization  
 1655       step, based on the known branching ratios.

## 1656       **3.2 Monte Carlo Event Generators.**

1657       The event generation described in the previous section has been implemented in  
 1658       several software packages for which a brief description is given.

- 1659     • **PYTHIA 8.** It is a program designed to perform the generation of high energy  
 1660        physics events which describes the collisions between particles such as electrons  
 1661        and protons. Several theories and models are implemented in it, in order to  
 1662        describe physical aspects like hard and soft interaction, parton distributions,  
 1663        initial and final-state parton showers, multiple parton interactions, beam rem-  
 1664        nants, hadronization<sup>2</sup> and particle decay. Thanks to extensive testing, several  
 1665        optimized parametrizations, known as *tunings*, have been defined in order to  
 1666        improve the description of actual collisions to a high degree of precision; for  
 1667        analysis at  $\sqrt{s} = 13$  TeV, the underline event CUETP8M1 tune is employed [97].  
 1668        The calculation of the matrix element is performed at LO which is not enough  
 1669        for the current required level of precision; therefore, pythia is often used for  
 1670        parton shower, hadronization and decays, while other event generators are used  
 1671        to generate the matrix element at NLO.
  
- 1672     • **MadGraph5\_aMC@NLO.** MadGraph is a matrix element generator which  
 1673        calculates the amplitudes for all contributing Feynman diagrams of a given  
 1674        process but does not provide a parton shower while MC@NLO incorporates  
 1675        NLO QCD matrix elements consistently into a parton shower framework; thus,  
 1676        MadGraph5\_aMC@NLO, as a merger of the two event generators MadGraph5  
 1677        and aMC@NLO, is an event generator capable to calculate tree-level and NLO  
 1678        cross sections and perform the matching of those with the parton shower. It is  
 1679        one of the most frequently used matrix element generators; however, it has the  
 1680        particular feature of the presence of negative event weights which reduce the  
 1681        number of events used to reproduce the properties of the objects generated [98].
  
- 1682     • **POWHEG.** It is an NLO matrix element generator where the hardest emis-

---

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

1683 sion of color charged particles is generated in such a way that the negative event  
 1684 weights issue of MadGraph5\_aMC@NLO is overcome; however, the method re-  
 1685 quires an interface with  $p_T$ -ordered parton shower or a parton shower generator  
 1686 where this highest emission can be vetoed in order to avoid double counting of  
 1687 this highest-energetic emission. PYTHIA is a commonly matched to POWHEG  
 1688 event generator [100].

1689 Events resulting from the whole generation process are known as MC events.

### 1690 3.3 CMS detector simulation.

1691 After generation, MC events contain the physics of the collisions but they are not  
 1692 ready to be compared to the events recorded by the experiment since these recorded  
 1693 events correspond to the response of the detection systems to the interaction with  
 1694 the particles traversing them. The simulation of the CMS detector has to be applied  
 1695 on top of the event generation; it is simulated with a MC toolkit for the simulation  
 1696 of particles passing through matter called Geant4 which is also able to simulate the  
 1697 electronic signals that would be measured by all detectors inside CMS.

1698 The simulation takes the generated particles contained in the MC events as input,  
 1699 makes them pass through the simulated geometry, and models physics processes that  
 1700 particles experience during their passage through matter. The full set of results from  
 1701 particle-matter interactions corresponds to the simulated hit which contains informa-  
 1702 tion about the energy loss, momentum and position. Particles of the input event are  
 1703 called *primary*, while the particles originating from GEANT4-modeled interactions of  
 1704 a primary particle with matter are called a *secondary*. Simulated hits are the input  
 1705 of subsequent modules that emulate the response of the detector readout system and

1706 triggers. The output from the emulated detection systems and triggers is known as  
 1707 digitization [101, 102].

1708 The modeling of the CMS detector corresponds to the accurate modeling of the  
 1709 interaction among particles, the detector material, and the magnetic field. This  
 1710 simulation procedure includes the following standard steps

1711 • Modeling of the Interaction Region.

1712 • Modeling of the particle passage through the hierarchy of volumes that compose  
 1713 CMS detector and of the accompanying physics processes.

1714 • Modeling of the effect of multiple interactions per beam crossing and/or the  
 1715 effect of events overlay ( Pile-Up simulation).

1716 • Modeling of the detector's electronics response, signal shape, noise, calibration  
 1717 constants (digitization).

1718 In addition to the full simulation, i.e., a detailed detector simulation, a faster  
 1719 simulation (FastSim) have been developed, that may be used where much larger  
 1720 statistics are required. In FastSim, detector material effects are parametrized and  
 1721 included in the hits; those hits are used as input of the same higher-level algorithms<sup>3</sup>  
 1722 used to analyze the recorded events. In this way, comparisons between fast and full  
 1723 simulations can be performed [104].

1724 After the full detector simulation, the output events can be directly compared  
 1725 to events actually recorded in the CMS detector. The collection of MC events that  
 1726 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

1727 **3.4 Event reconstruction.**

1728 The CMS experiment use the *particle-flow event reconstruction algorithm (PF)* to do  
1729 the reconstruction of particles produced in  $pp$  collisions. Next sections will present  
1730 a basic description of the *Elements* used by PF (tracker tracks, energy clusters, and  
1731 muon tracks), based in the References [105, 106] where more detailed descriptions can  
1732 be found.

1733 **3.4.1 Particle-Flow Algorithm.**

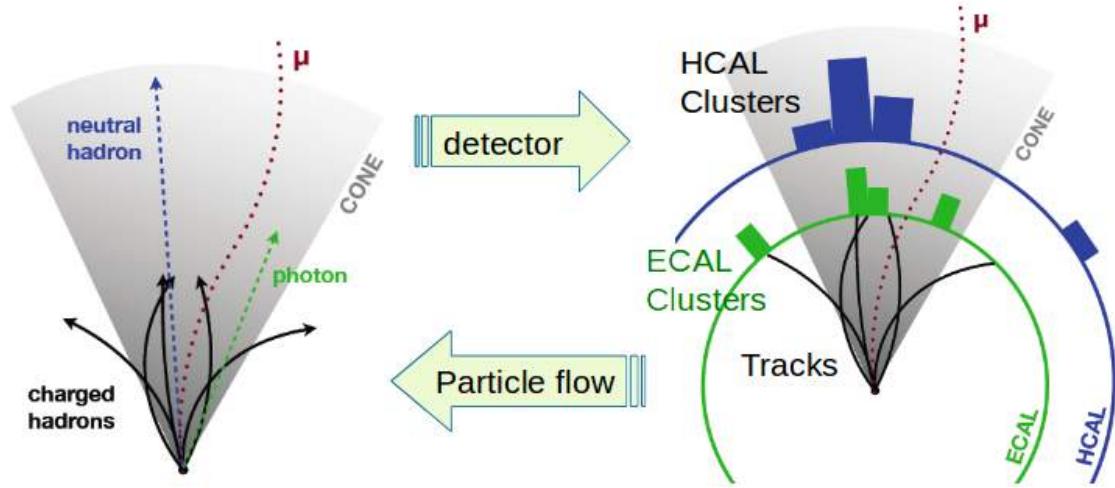
1734 Each of the several sub detection systems of the CMS detector is dedicated to identify  
1735 an specific type of particles, i.e., photons and electrons are absorbed by the ECAL  
1736 and their reconstruction is based on ECAL information; hadrons are reconstructed  
1737 from clusters in the HCAL while muons are reconstructed from hits in the muon  
1738 chambers. PF is designed to correlate signals from all the detector layers (tracks and  
1739 energy clusters) in order to reconstruct and identify each final state particle and its  
1740 properties as sketched in Figure 3.2.

1741 For instance, a charged hadron is identified by a geometrical connection, known  
1742 as *link*, between one or more calorimeter clusters and a track in the tracker, provided  
1743 there are no hits in the muon system; combining several measurements allows a better  
1744 determination of the energy and charge sign of the charged hadron.

1745 **Charged-particle track reconstruction.**

1746 The strategy used by PF in order to reconstruct tracks is called *Iterative Tracking*  
1747 which occurs in four steps

- 1748 • Seed generation where initial track candidates are found by looking for a combi-  
1749 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].

1750 ten iterations are performed, each one with a different seeding requirement.  
 1751 Seeds are used to estimate the trajectory parameters and uncertainties at the  
 1752 time of the full track reconstruction. Seeds are also considered track candidates.

- 1753 • Track finding using a tracking software known as Combinatorial Track Finder  
 1754 (CTF) [108]. The seed trajectories are extrapolated along the expected flight  
 1755 path of a charged particle, in agreement to the trajectory parameters obtained  
 1756 in the first step, in an attempt to find additional hits that can be assigned to  
 1757 the track candidates.
  - 1758 • Track-fitting where the found tracks are passed as input to a module which  
 1759 provides the best estimate of the parameters of each trajectory.
  - 1760 • Track selection where track candidates are submitted to a selection which dis-  
 1761 cards those that fail a set of defined quality criteria.
- 1762 Iterations differ in the seeding configuration and the final track selection as elab-

1763 orated in References [105, 106]. In the first iteration, high  $p_T$  tracks and tracks pro-  
 1764 duced near to the interaction region are identified and those hits are masked thereby  
 1765 reducing the combinatorial complexity. Next, iterations search for more complicated  
 1766 tracks, like low  $p_T$  tracks and tracks from b hadron decays, which tend to be displaced  
 1767 from the interaction region.

1768 **Vertex reconstruction.**

1769 During the track reconstruction, an extrapolation toward to the calorimeters is per-  
 1770 formed in order to match energy deposits; that extrapolation is performed also toward  
 1771 the beamline in order to find the origin of the track known as *vertex*. The vertex re-  
 1772 construction is performed by selecting from the available reconstructed tracks, those  
 1773 that are consistent with being originated in the interaction region where  $pp$  collisions  
 1774 are produced. The selection involves a requirement on the number of tracker (pixel  
 1775 and strip) hits and the goodness of the track fit.

1776 Selected tracks are clustered using a *deterministic annealing algorithm* (DA)<sup>4</sup>. A  
 1777 set of candidate vertices and their associated tracks, resulting from the DA, are then  
 1778 fitted with an *adaptive vertex fitter* (AVF) to produce the best estimate of the vertices  
 1779 locations.

1780 The  $p_T$  of the tracks associated to a reconstructed vertex is added, squared and  
 1781 used to organize the vertices; the vertex with the highest squared sum is designated  
 1782 as the *primary vertex* (*PV*) while the rest are designated as PU vertices.

1783 **Calorimeter clustering.**

1784 After traversing the CMS tracker system, electrons, photons and hadrons deposit their  
 1785 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]

1786 a high detection efficiency even for low-energy particles and an efficient distinction  
 1787 between close energy deposits. The clustering runs independently in the ECAL barrel  
 1788 and endcaps, HCAL barrel and endcaps, and the two preshower layers, following two  
 1789 steps

- 1790     • cells with an energy larger than a given seed threshold and larger than the energy  
     1791        of the neighboring cells are identified as cluster seeds. The neighbor cells are  
     1792        those that either share a side with the cluster seed candidate, or the eight closest  
     1793        cells including cells that only share a corner with the seed candidate.
- 1794     • cells with at least a corner in common with a cell already in the cluster seed  
     1795        and with an energy above a cell threshold are grouped into topological clusters.

1796 Clusters formed in this way are known as *particle-flow clusters*. With this cluster-  
 1797 ing strategy, it is possible to detect and measure the energy and direction of photons  
 1798 and neutral hadrons as well as differentiate these neutral particles from the charged  
 1799 hadron energy deposits. In cases involving charged hadrons for which the track pa-  
 1800 rameters are not determined accurately, for instance, low-quality and high- $p_T$  tracks,  
 1801 clustering helps in the energy measurements.

## 1802 Electron track reconstruction.

1803 Although the charged-particle track reconstruction described above works for elec-  
 1804 trons, they lose a significant fraction of their energy via bremsstrahlung photon radi-  
 1805 ation before reaching the ECAL; thus, the reconstruction performance depends on the  
 1806 ability to measure also the radiated energy. The reconstruction strategy, in this case,  
 1807 requires information from the tracking system and from the ECAL. Bremsstrahlung  
 1808 photons are emitted at similar  $\eta$  values to that of the electron but at different values  
 1809 of  $\phi$ ; therefore, the radiated energy can be recovered by grouping ECAL clusters in a

1810  $\eta$  window over a range of  $\phi$  around the electron direction. The group is called ECAL  
 1811 supercluster.

1812 Electron candidates from the track-seeding and ECAL super clustering are merged  
 1813 into a single collection which is submitted to a full electron tracking fit with a  
 1814 Gaussian-sum filter (GSF) [109]. The electron track and its associated ECAL su-  
 1815 percluster form a *particle-flow electron*.

### 1816 Muon track reconstruction.

1817 Given that the CMS detector is equipped with a muon spectrometer capable to iden-  
 1818 tify and measure the momentum of the muons traversing it, the muon reconstruction  
 1819 is not specific to PF; therefore, three different muon types are defined

- 1820     ● *Standalone muon.* A clustering on the DTs or CSCs hits is performed to form  
 1821       track segments; those segments are used as seeds for the reconstruction in the  
 1822       muon spectrometer. All DTs, CSCs, and RPCs hits along the muon trajectory  
 1823       are combined and fitted to form the full track. The fitting output is called a  
 1824       *standalone-muon track*.
- 1825     ● *Tracker muon.* Each track in the inner tracker with  $p_T$  larger than 0.5 GeV and  
 1826       a total momentum  $p$  larger than 2.5 GeV is extrapolated to the muon system.  
 1827       A *tracker muon track* corresponds to a extrapolated track that matches at least  
 1828       one muon segment.
- 1829     ● *Global muon.* When tracks in the inner tracker (inner tracks) and standalone-  
 1830       muon tracks are matched and turn out being compatibles, their hits are com-  
 1831       bined and fitted to form a *global-muon track*.

1832        Global muons sharing the same inner track with tracker muons are merged into  
 1833      a single candidate. PF muon identification uses the muon energy deposits in ECAL,  
 1834      HCAL, and HO associated with the muon track to improve the muon identification.

1835 **Particle identification and reconstruction.**

1836      PF elements are connected by a linker algorithm that tests the connection between any  
 1837      pair of elements; if they are found to be linked, a geometrical distance that quantifies  
 1838      the quality of the link is assigned. Two elements may be linked indirectly through  
 1839      common elements. Linked elements form *PF blocks* and each PF block may contain  
 1840      elements originating in one or more particles. Links can be established between  
 1841      tracks, between calorimeter clusters, and between tracks and calorimeter clusters.  
 1842      The identification and reconstruction start with a PF block and proceed as follows

1843        • Muons. An *isolated global muon* is identified by evaluating the presence of  
 1844      inner track and energy deposits close to the global muon track in the  $(\eta, \phi)$   
 1845      plane, i.e., in a particular point of the global muon track, inner tracks and  
 1846      energy deposits are sought within a radius of  $\Delta R = 0.3$  (see eqn. 2.7) from the  
 1847      muon track; if they exist and the  $p_T$  of the found track added to the  $E_T$  of the  
 1848      found energy deposit does not exceed 10% of the muon  $p_T$  then the global muon  
 1849      is an isolated global muon. This isolation condition is stringent enough to reject  
 1850      hadrons misidentified as muons.

1851        *Non-isolated global muons* are identified using additional selection requirements  
 1852      on the number of track segments in the muon system and energy deposits along  
 1853      the muon track. Muons inside jets are identified with more stringent criteria  
 1854      in isolation and momentum as described in Reference [112]. The PF elements  
 1855      associated with an identified muon are masked from the PF block.

- 1856     ● Electrons are identified and reconstructed as described above plus some addi-  
 1857         tional requirements on fourteen variables like the amount of energy radiated,  
 1858         the distance between the extrapolated track position at the ECAL and the po-  
 1859         sition of the associated ECAL supercluster, among others, which are combined  
 1860         in an specialized multivariate analysis strategy that improves the electron iden-  
 1861         tification. Tracks and clusters used to identify and reconstruct electrons are  
 1862         masked in the PF block.
- 1863     ● Isolated photons are identified from ECAL superclusters with  $E_T$  larger than 10  
 1864         GeV, for which the energy deposited at a distance of 0.15, from the supercluster  
 1865         position on the  $(\eta, \phi)$  plane, does not exceed 10% of the supercluster energy;  
 1866         note that this is an isolation requirement. In addition, there must not be links  
 1867         to tracks. Clusters involved in the identification and reconstruction are masked  
 1868         in the PF block.
- 1869     ● Bremsstrahlung photons and prompt photons tend to convert to electron-positron  
 1870         pairs inside the tracker, therefore, a dedicated finder algorithm is used to link  
 1871         tracks that seem to originate from a photon conversion; in case those two tracks  
 1872         are compatible with the direction of a bremsstrahlung photon, they are also  
 1873         linked to the original electron track. Photon conversion tracks are also masked  
 1874         in the PF block.
- 1875     ● The remaining elements in the PF block are used to identify hadrons. In the  
 1876         region  $|\eta| \leq 2.5$ , neutral hadrons are identified with HCAL clusters not linked  
 1877         to any track while photons from neutral pion decays are identified with ECAL  
 1878         clusters without links to tracks. In the region  $|\eta| > 2.5$  ECAL clusters linked to  
 1879         HCAL clusters are identified with a charged or neutral hadron shower; ECAL  
 1880         clusters with no links are identified with photons. HCAL clusters not used yet,

1881       are linked to one or more unlinked tracks and to an unlinked ECAL in order to  
 1882       reconstruct charged-hadrons or a combination of photons and neutral hadrons  
 1883       according to certain conditions on the calibrated calorimetric energy.

- 1884       • Charged-particle tracks may be liked together when they converge to a *sec-*  
 1885       *ondary vertex (SV)* displaced from the IP where the PV and PU vertices are  
 1886       reconstructed; at least three tracks are needed in that case, of which at most  
 1887       one has to be an incoming track with hits in tracker region between a PV and  
 1888       the SV.

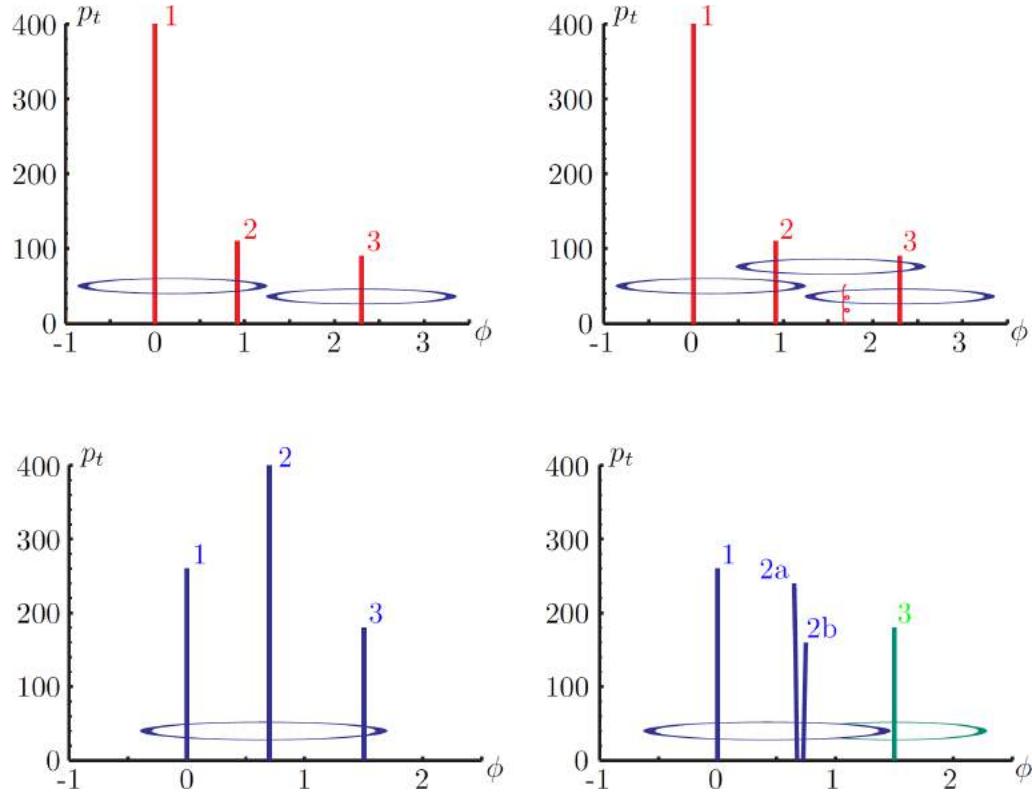
1889       The linker algorithm, as well as the whole PF algorithm, has been validated and  
 1890       commissioned; results from that validation are presented in the Reference [105].

1891 **Jet reconstruction.**

1892       Quarks and gluons may be produced in the  $pp$  collisions, therefore, their hadronization  
 1893       will be seen in the detector as a shower of hadrons and their decay products in the  
 1894       form of a *jet*. Two classes of clustering algorithms have been developed based in  
 1895       their jet definition [113]:

- 1896       • Iterative cone algorithms (IC). Jets are defined in terms of circles of fixed radius  
 1897        $R$  in the  $\eta\text{-}\phi$  plane, known as *stable cones*, for which the sum of the momenta  
 1898       of all the particles within the cone points in the same direction as the center  
 1899       of the circle. The seed of the iteration is the hardest non-isolated particle in  
 1900       the event, then, the resulting momentum direction is assigned as the new cone  
 1901       direction and a new iteration starts; iteration process stops when the cone if  
 1902       found to be stable.

1903     • Sequential recombination algorithms. The distance between non-isolated par-  
 1904        ticles is calculated; if that distance is below a threshold, these particles are  
 1905        recombined into a new object. The sequence is repeated until the separation  
 1906        between the recombined object and any other particle is above certain thresh-  
 1907        old; the recombined object is called a jet and the algorithm starts again with  
 1908        the remaining particles.



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

1909        Two conditions are of particular importance for the clustering algorithms, *infrared*  
 1910        and *collinear (IRC) safety*. In order to explain the concept of infrared (IR) safety,  
 1911        consider an event with three hard particles as shown in the top left side of Figure 3.3,  
 1912        two stable cones are found and then two jets are identified; if a soft gluon is added, as  
 1913        shown in the top right side of Figure 3.3, three stable cones are found and the three

1914 hard particles are now clustered into a single jet. If the addition of soft particles  
 1915 change the outcome of the clustering, then it is said that the algorithm is IR unsafe.  
 1916 Soft radiation is highly likely in perturbative QCD, which dominates the physics of  
 1917 the jets, and then IR unsafe effect leads to divergences [113].

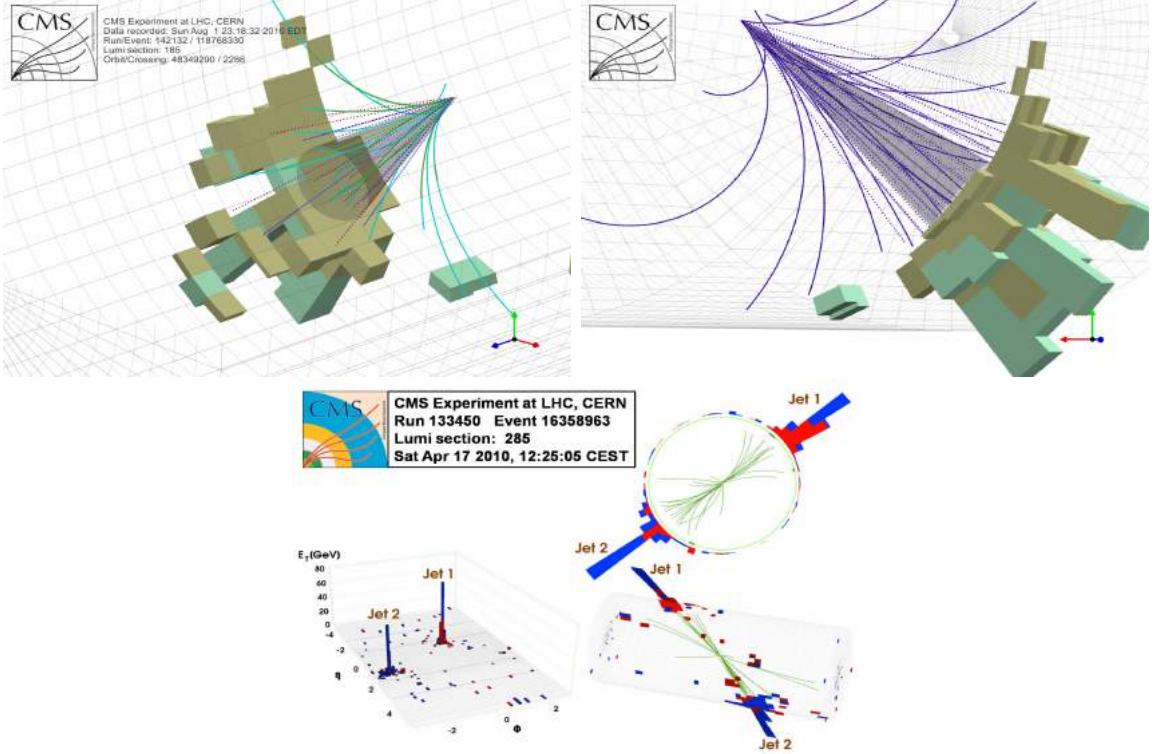
1918 The concept of collinear safety can also be explained considering a three hard  
 1919 particles event, as shown in the bottom left side of Figure 3.3, where one stable cone  
 1920 containing all three particles is found and one jet is identified; if the hardest particle  
 1921 is split into two collinear particles (2a and 2b) in the bottom right side of Figure 3.3,  
 1922 then the clustering results in a different jet identification and the algorithm is said  
 1923 to be collinear unsafe. The collinear unsafe effect leads to divergences in jet cross  
 1924 section calculations [114].

1925 It has been determined that IC algorithms are IRC unsafe, and therefore, they  
 1926 have to be replaced by algorithms that not only provide the finite perturbative results  
 1927 from theoretical computations, but also that are not highly dependent on underlying  
 1928 event and pileup effects which leads to significant corrections [113].

1929 The sequential recombination algorithms arise as the IRC safe alternative used by  
 1930 the CMS experiment; in particular the anti- $k_t$  algorithm which is a generalization of  
 1931 the previously existing  $k_t$  [115] and Cambridge/Aachen [116] jet clustering algorithms.

1932 The anti- $k_t$  algorithm is used to perform the jet reconstruction by clustering those  
 1933 PF particles within a cone (see Figure 3.4); previously, isolated electrons, isolated  
 1934 muons, and charged particles associated with other interaction vertices are excluded  
 1935 from the clustering.

1936 The anti- $k_t$  algorithm proceeds in a sequential recombination of PF particles; the  
 1937 distance between particles  $i$  and  $j$  ( $d_{ij}$ ) and the distance between particles and the  
 1938 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].

$$\begin{aligned}
 d_{ij} &= \min\left(\frac{1}{k_{ti}^2}, \frac{1}{k_{tj}^2}\right) \frac{\Delta_{ij}^2}{R^2} \\
 d_{iB} &= \frac{1}{k_{ti}^2}
 \end{aligned} \tag{3.1}$$

1939 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, 1940 rapidity and azimuth of particle  $i$  respectively and  $R$  is the called jet radius. For all 1941 the remaining PF particles, after removing the isolated ones,  $d_{ij}$  and  $d_{iB}$  are calcu-

1942 lated<sup>5</sup> and the smallest is identified; if it is a  $d_{ij}$ , particles  $i$  and  $j$  are replaced with  
 1943 a new object whose momentum is the vectorial sum of the combined particles. If the  
 1944 smallest distance is a  $d_{iB}$  the clustering process ends, the object  $i$  (which at this stage  
 1945 should be a combination of several PF particles) is declared as a *Particle-flow-jet* (PF  
 1946 jet) and all the associated PF particles are removed from the detector. The clustering  
 1947 process is repeated until no PF particles remain.  $R$  is a free parameter that can be  
 1948 adjusted according to the specific analysis conditions; usually, two values are used,  
 1949  $R=0.4$  and  $R=0.5$ , giving the name to the so-called AK4-jet and AK5-jet respectively.

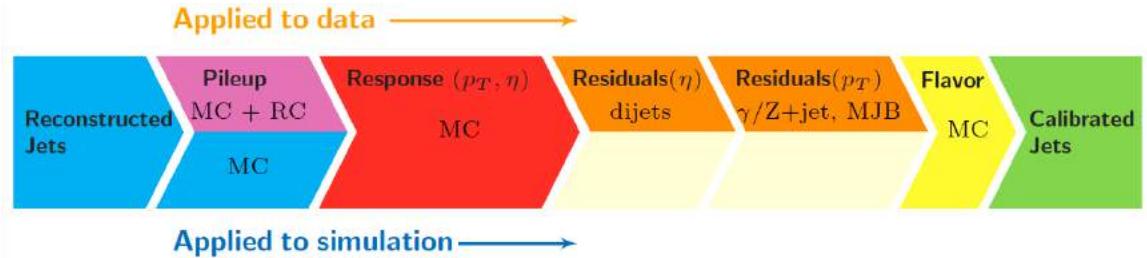
1950 An advantage of the anti- $k_t$  algorithm over other clustering algorithms is the reg-  
 1951 ularity of the boundaries of the resulting jets. For all known IRC safe algorithms,  
 1952 soft radiation can introduce irregularities in the boundaries of the final jets; however,  
 1953 anti- $k_t$  algorithm is soft-resilient, meaning that jets shape is not affected by soft radi-  
 1954 ation, which is a valuable property considering that knowing the typical shape of jets  
 1955 makes experimental calibration of jets more simple. In addition, that soft-resilience  
 1956 is expected to simplify certain theoretical calculations and reduce the momentum-  
 1957 resolution loss caused by underlying-event (UE) and pileup contamination [114].

1958 The effect of the UE and pileup contamination over a jet identification, can be  
 1959 seen as if soft events are added to the jet; for instance, if a soft event representing UE  
 1960 or pileup is added to an event for which a set of jets  $J$  have been identified, and the  
 1961 clustering is rerun on that new extended event, the outcome will be different in two  
 1962 aspects: jets will contain some additional soft energy and the distribution of particles  
 1963 in jets may have change; that effect is called *back-reaction*. The back-reaction effect in  
 1964 the anti- $k_t$  algorithm is suppressed not by the amount of momentum added to the jet  
 1965 but by the jet transverse momentum  $p_{T,J}$ , which means that this strong suppression  
 1966 leads to a smaller correction due to EU and pileup effect [114].

---

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

1967 Jet energy Corrections



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

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

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

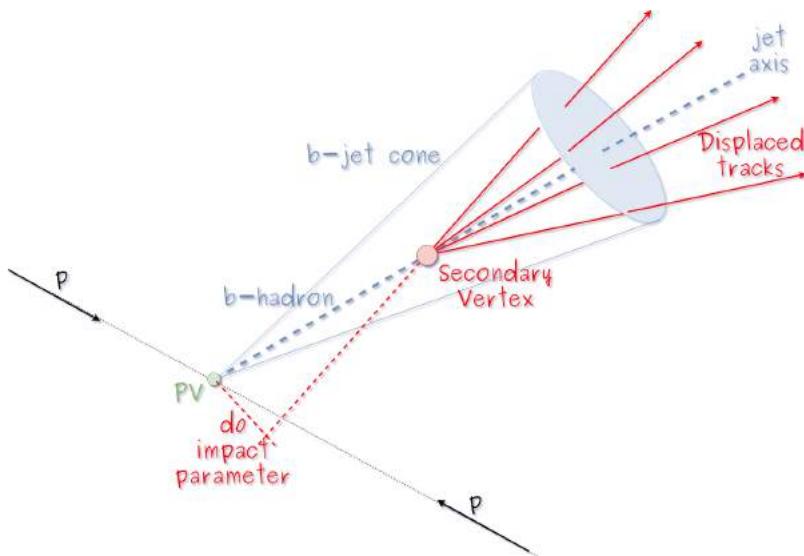
- Level 1 correction removes the energy coming from pile-up. The scale factor is determined using a MC sample of QCD dijet (2 jets) events with and without pileup overlay; it is parametrized in terms of the offset energy density  $\rho$ , jet area  $A$ , jet  $\eta$  and jet  $p_T$ . Different corrections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

1985 barrel reference region. The Residuals  $p_T$ -dependent correct the jet absolute  
 1986 scale (JES vs  $p_T$ ).

- 1987 • Jet-flavor corrections are derived in the same way as MC-truth corrections but  
 1988 using QCD pure flavor samples.

1989 ***b*-tagging of jets.**

1990 A particular feature of the hadrons containing bottom quarks (*b*-hadrons) is that  
 1991 their lifetime is long enough to travel some distance before decaying, but it is not as  
 1992 long as those of light quark hadrons; therefore, when looking at the hadrons produced  
 1993 in  $pp$  collisions, *b*-hadrons decay typically inside the tracker rather than reaching the  
 1994 calorimeters as some light-hadrons do. As a result, a *b*-hadron decay gives rise to a  
 1995 displaced vertex (secondary vertex) with respect to the primary vertex as shown in  
 1996 Figure 3.6; the SV displacement is in the order of a few millimeters. A jet resulting  
 1997 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.

1998 Several methods to identify *b*-jets (*b*-tagging) have been developed; the method

1999 used in this thesis is known as *Combined Secondary Vertex* algorithm in its second  
 2000 version (CSVv2) [121]. By using information of the impact parameter, the recon-  
 2001 structed secondary vertices, and the jet kinematics as input in a multivariate analysis  
 2002 that combines the discrimination power of each variable in one global discrimina-  
 2003 tor variable, three working points (references): loose, medium and tight, are defined  
 2004 which quantify the probabilities of mistag jets from light quarks as jets from  $b$  quarks;  
 2005 10, 1 and 0.1 % respectively. Although the mistagging probability decreases with the  
 2006 working point strength, the efficiency to correctly tag  $b$ -jets also decreases as 83, 69  
 2007 and 49 % for the respective working point; therefore, a balance needs to be achieved  
 2008 according to the specific requirements of the analysis.

2009 **Missing transverse energy.**

2010 The fact that proton bunches carry momentum along the  $z$ -axis implies that for  
 2011 each event it is expected that the momentum in the transverse plane is balanced.  
 2012 Imbalances are quantified by the missing transverse energy (MET) and are attributed  
 2013 to several sources including particles escaping undetected through the beam pipe,  
 2014 neutrinos produced in weak interactions processes which do not interact with the  
 2015 detector and thus escaping without leaving a sign, or even undiscovered particles  
 2016 predicted by models beyond the SM.

2017 The PF algorithm assigns the negative sum of the momenta of all reconstructed  
 2018 PF particles to the *particle-flow MET* according to

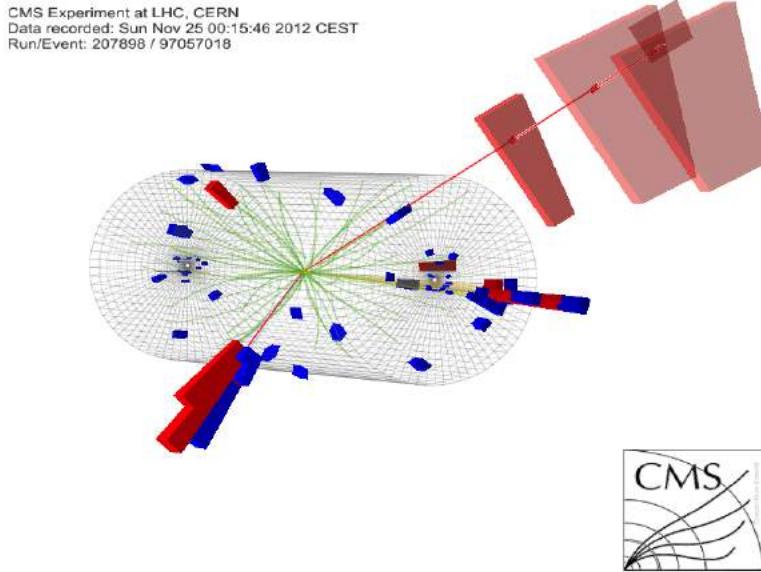
$$\vec{E}_T = - \sum_i \vec{p}_{T,i} \quad (3.2)$$

2019 JEC are propagated to the calculation of the  $\vec{E}_T$  as described in the Reference [122].

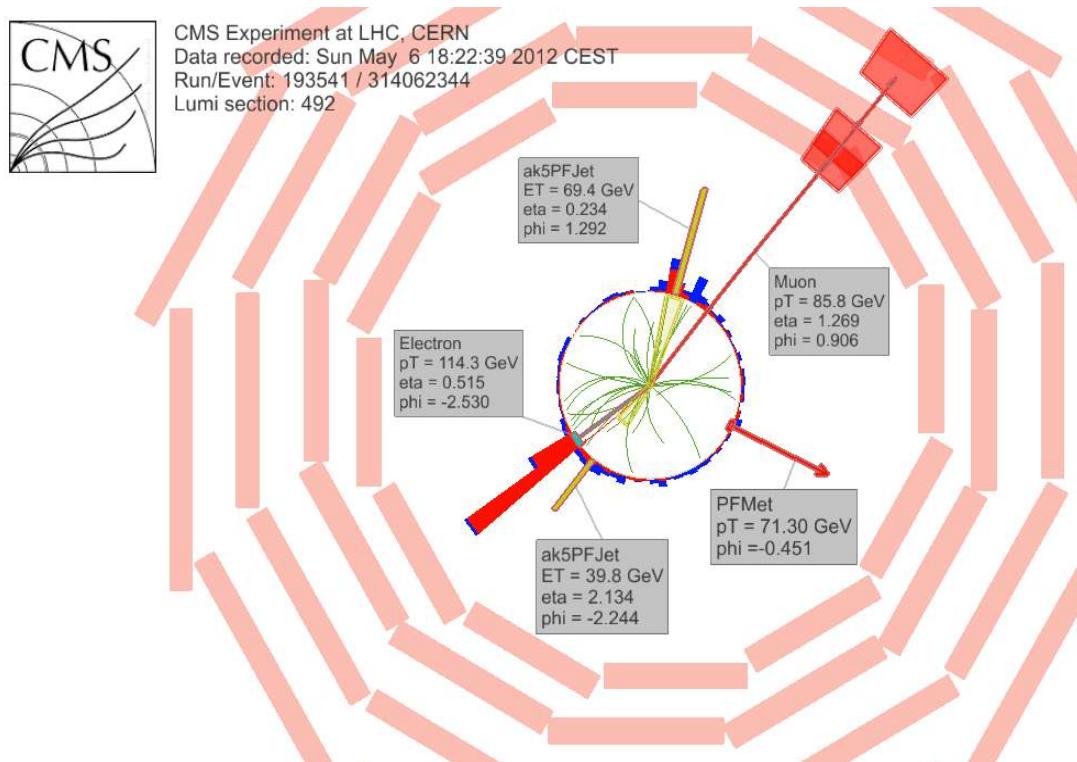
2020 **3.4.2 Event reconstruction examples**

2021 Figures 3.7-3.9 show the results of the reconstruction performed on 3 recorded events.

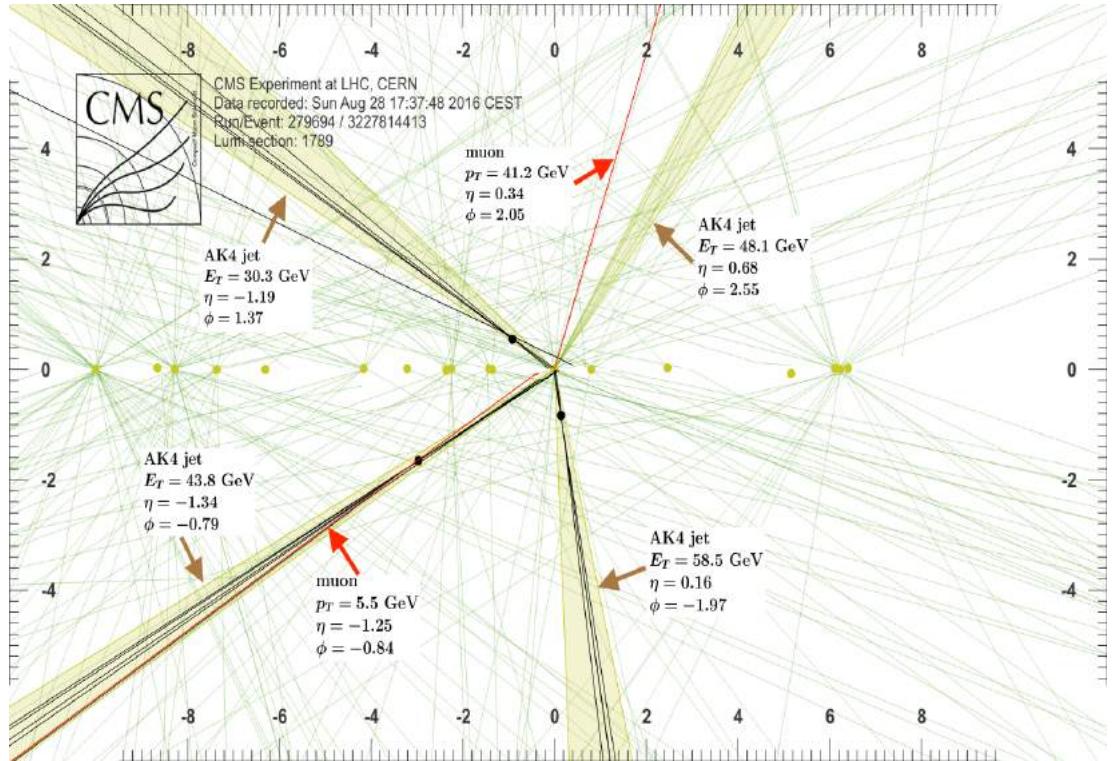
2022 Descriptions are taken directly from the source.



**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].

2023 **Chapter 5**

2024 **Statistical methods**

2025 In the course of analyzing the data sets provided by the CMS experiment and used in  
2026 this thesis, several statistical tools have been employed; in this chapter, a description  
2027 of these tools will be presented, starting with the general statement of the multivariate  
2028 analysis methods, followed by the particularities of the Boosted Decision Trees (BDT)  
2029 method and its application to the classification problem. Statistical inference methods  
2030 used will also be presented. This chapter is based mainly on References [126–128].

2031 **5.1 Multivariate analysis**

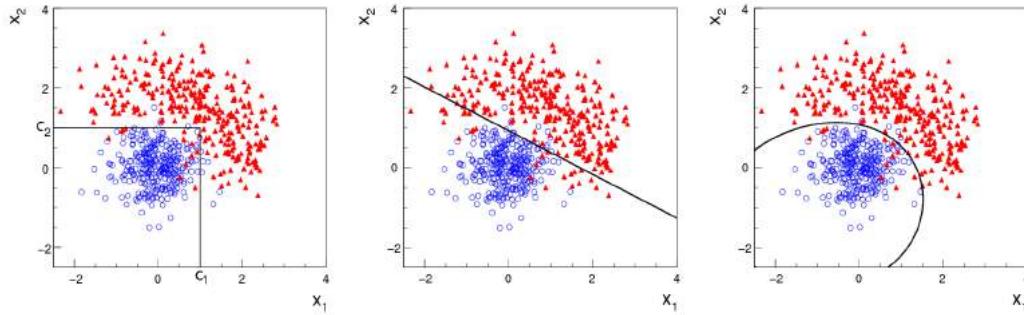
2032 Multivariate data analysis (MVA) makes use of the statistical techniques developed to  
2033 analyze more than one variable at once, taking into account all the correlations among  
2034 variables. MVA is employed in a variety of fields like consumer and market research,  
2035 quality control and process optimization. Using MVA it is possible to identify the  
2036 dominant patterns in a data sample, like groups, outliers and trends, and determine  
2037 to which group a set of values belong; in the particle physics context, MVA methods  
2038 are used to perform the selection of certain type of events from a large data set.

2039        Processes with small cross section, such as the  $tHq$  process ( $\sigma_{SM}(\sqrt{s} = 13\text{TeV}) =$   
 2040      70.96 fb), are hard to detect in the presence of the processes with larger cross sections,  
 2041       $\sigma_{SM}^{t\bar{t}}(\sqrt{s} = 13\text{TeV}) = 823.44$  fb for instance; therefore, only a small fraction of the data  
 2042      contains events of interest (signal), the major part is signal-like events, which mimic  
 2043      signal characteristics but belong to different processes, so they are a background to  
 2044      the process of interest. This implies that it is not possible to say with certainty  
 2045      that a given event is a signal or a background and statistical methods should be  
 2046      involved. In that sense, the challenge can be formulated as one where a set of events  
 2047      have to be classified according to certain special features; these features correspond  
 2048      to the measurements of several parameters like energy or momentum, organized in a  
 2049      set of *input variables*. The measurements for each event can be written in a vector  
 2050       $\mathbf{x} = (x_1, \dots, x_n)$  for which

- 2051        •  $f(\mathbf{x}|s)$  is the probability density (*likelihood function*) that  $\mathbf{x}$  is the set of mea-  
 2052        sured values given that the event is a signal event (signal hypothesis).
- 2053        •  $f(\mathbf{x}|b)$  is the probability density (*likelihood function*) that  $\mathbf{x}$  is the set of mea-  
 2054        sured values given that the event is a background event (background hypothe-  
 2055        sis).

2056        Figure 5.1 shows three ways to perform a classification of events for which mea-  
 2057        surements of two properties, i.e., two input variables  $x_1$  and  $x_2$ , have been performed;  
 2058        blue circles represent signal events while red triangles represent background events.  
 2059        The classification on the left is *cut-based* requiring  $x_1 < c_1$  and  $x_2 < c_2$ ; usually the  
 2060        cut values ( $c_1$  and  $c_2$ ) are chosen according to some knowledge about the event pro-  
 2061        cess. In the middle plot, the classification is performed using a linear function of  
 2062        the input variables, hence the boundary is a straight line, while in the right plot the

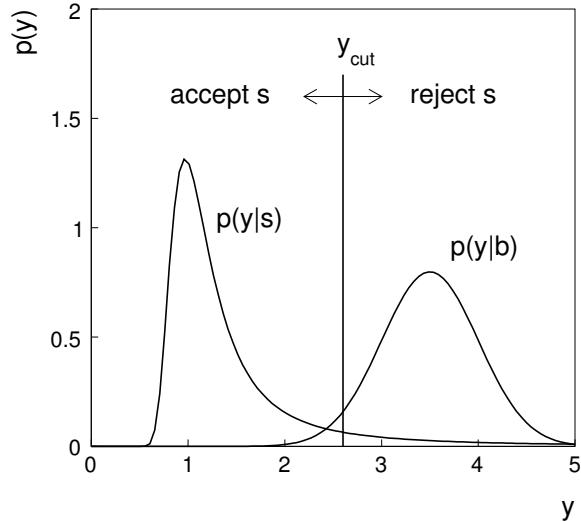
2063 the relationship between input variables is not linear thus the boundary is not linear  
 2064 either.



**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]

2065 In general, the boundary can be parametrized in terms of the input variables such  
 2066 that the cut is set on the parametrization instead of on the variables, i.e.,  $y(\mathbf{x}) = y_{cut}$   
 2067 with  $y_{cut}$  being a constant; thus, the acceptance or rejection of an event is based on  
 2068 which side of the boundary the event is located. If  $y(\mathbf{x})$ , usually called *test statistic*,  
 2069 has functional form, it can be used to determine the probability distribution functions  
 2070  $p(y|s)$  and  $p(y|b)$  and then perform a test statistic with a single cut on the scalar  
 2071 variable  $y$ .

2072 Figure 5.2 shows an example of what would be the probability distribution func-  
 2073 tions under the signal and background hypotheses for a scalar test statistic with a cut  
 2074 on the classifier  $y$ . Note that the tails of the distributions indicate that some signal  
 2075 events fall in the rejection region and some background events fall on the acceptance  
 2076 region; therefore, it is convenient to define the *efficiency* with which events of a given  
 2077 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]

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

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

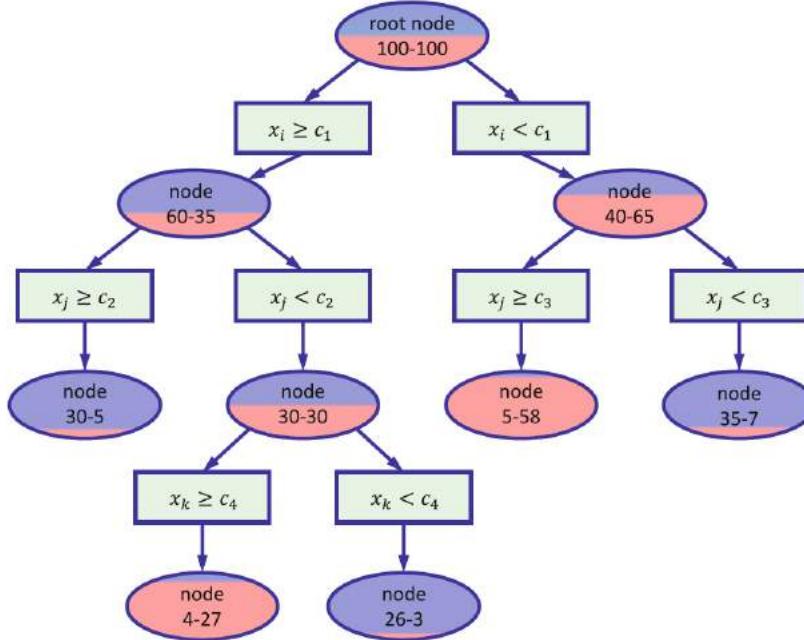
2078 where  $A$  is the acceptance region. If the background hypothesis is the *null hypothesis*  
 2079 ( $H_0$ ), the signal hypothesis would be *alternative hypothesis* ( $H_1$ ); in this context, the  
 2080 background efficiency corresponds to the significance level of the test ( $\alpha$ ) and describes  
 2081 the misidentification probability, while the signal efficiency corresponds to the power  
 2082 of the test ( $1-\beta$ )<sup>1</sup> and describes the probability of rejecting the background hypothesis  
 2083 if the signal hypothesis is true. What is sought in an analysis is to maximize the power  
 2084 of the test relative to the significance level, i.e., set a selection with the largest possible  
 2085 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

2086 **5.1.1 Decision trees**

2087 For this thesis, the implementation of the MVA strategy, described above, is per-  
 2088 formed through decision trees by using the TMVA software package [127] included  
 2089 in the ROOT analysis framework [129]. In a simple picture, a decision tree classifies  
 2090 events according to their input variables values by setting a cut on each input variable  
 2091 and checking which events are on which side of the cut, just as proposed in the MVA  
 2092 strategy, but in addition, as a machine learning algorithm, decision trees offer the  
 2093 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].

2094 The training or growing of a decision tree is the process where the rules for clas-  
 2095 sifying events are defined; this process is represented in Figure 5.3 and consists of  
 2096 several steps:

- 2097 • take MC samples of signal and background events and split them into two parts

2098 each; the first parts will be used in the decision tree training, while the second  
 2099 parts will be used for testing the final classifier obtained from the training.  
 2100 Each event has associated a set of input variables  $\mathbf{x} = (x_1, \dots, x_n)$  which serve  
 2101 to distinguish between signal and background events. The training sample is  
 2102 taken in at the *root node*.

- 2103     • Pick one variable, say  $x_i$ .
- 2104     • Pick one value of  $x_i$ , each event has its own value of  $x_i$ , and split the training  
     2105       sample into two subsamples  $B_1$  and  $B_2$ ;  $B_1$  contains events for which  $x_i < c_1$   
     2106       while  $B_2$  contains the rest of the training events;
- 2107     • scan all possible values of  $x_i$  and find the splitting value that provides the *best*  
     2108       classification<sup>2</sup>, i.e.,  $B_1$  is mostly made of signal events while  $B_2$  is mostly made  
     2109       of background events.
- 2110     • It is possible that variables other than the picked one produce a better classi-  
     2111       fication, hence, all the variables have to be evaluated. Pick the next variable,  
     2112       say  $x_j$ , and repeat the scan over its possible values.
- 2113     • At the end, all the variables and their values will have been scanned, the *best*  
     2114       variable and splitting value will have been identified, say  $x_1, c_1$ , and there will  
     2115       be two nodes fed with the subsamples  $B_1$  and  $B_2$ .

2116       Nodes are further split by repeating the decision process until a given number of  
 2117       final nodes is obtained, nodes are largely dominated by either signal or background  
 2118       events, or nodes have too few events to continue. Final nodes are called *leaves* and  
 2119       they are classified as signal or background leaves according to the class of the majority  
 2120       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.

2121        The quality of the classification at each node is evaluated through a separation  
 2122        criteria; there are several of them but the *Gini Index* ( $G$ ) is the one used in the  
 2123        decision trees trained for the analysis in this thesis.  $G$  is written in terms of the  
 2124        purity ( $P$ ), i.e., the fraction of signal events in the samples after the separation is  
 2125        made; it is given by

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

2126        note that  $P=0.5$  at the root node while  $G=0$  for pure leaves. For a node  $A$  split into  
 2127        two nodes  $B_1$  and  $B_2$  the  $G$  gain is

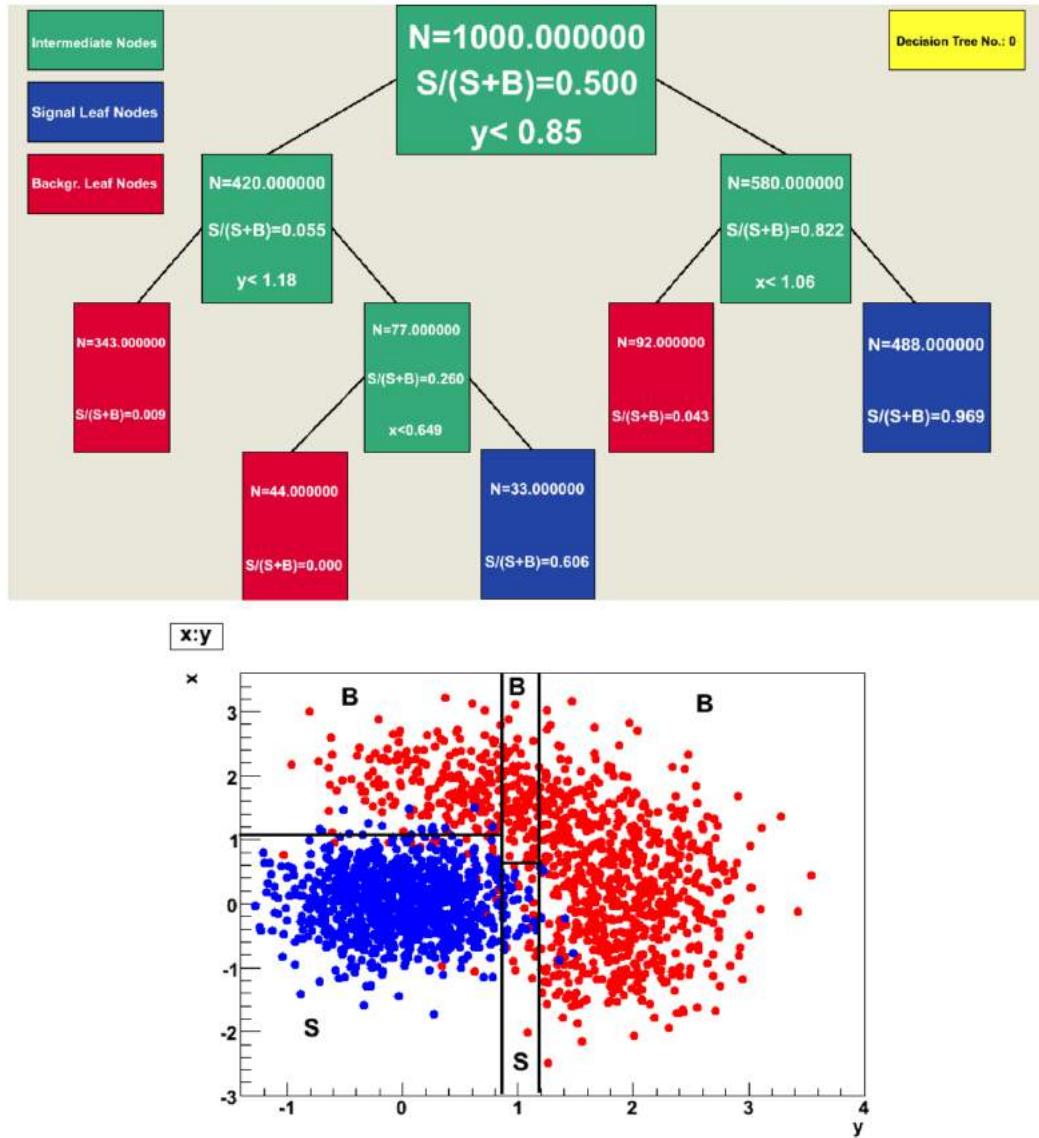
$$\Delta G = G(A) - G(B_1) - G(B_2). \quad (5.4)$$

2128        The *best* classification corresponds to that for which the gain of  $G$  is maximized;  
 2129        hence, the scanning over all the variables in an event and their values is of great  
 2130        importance.

2131        In order to provide a numerical output for the classification, events in a sig-  
 2132        nal(background) leaf are assigned an score of 1(-1) each, defining in this way the  
 2133        decision tree *classifier/weak learner* as

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

2134        Figure 5.4 shows an example of the classification of a sample of events, containing  
 2135        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].

### 2136 5.1.2 Boosted decision trees (BDT).

2137 Event misclassification occurs when a training event ends up in the wrong leaf, i.e., a  
 2138 signal event ends up in a background leaf or a background event ends up in a signal  
 2139 leaf. A way to correct it is to assign a weight to the misclassified events and train  
 2140 a second tree using the reweighted events; the event reweighting is performed by a

2141 boosting algorithm in such a way that when used in the training of a new decision  
 2142 tree the *boosted events* get correctly classified. The process is repeated iteratively  
 2143 adding a new tree to the forest and creating a set of classifiers, which are combined  
 2144 to create the next classifier; the final classifier offers more stability<sup>3</sup> and has a smaller  
 2145 misclassification rate than any individual ones. The resulting tree collection is known  
 2146 as a *boosted decision tree (BDT)*.

2147 Thus, purity of the sample is generalized to

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

2148 where  $w_s$  and  $w_b$  are the weights of the signal and background events respectively;  
 2149 the Gini index is also generalized

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

2150 with  $n$  the number of events in the node. The final score of an event, after pass-  
 2151 ing through the forest, is calculated as the renormalized sum of all the individual  
 2152 (possibly weighted) scores; thus, high(low) score implies that the event is most likely  
 2153 signal(background).

2154 The boosting procedure, implemented in the *Gradient boosting* algorithm used in  
 2155 this thesis, produces a classifier  $F(\mathbf{x})$  which is the weighted sum of the individual  
 2156 classifiers obtained after each iteration, i.e.,

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

2157 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.

2158 deviation between the classifier  $F(\mathbf{x})$  response and the true value  $y$  obtained from the  
 2159 training sample (1 for signal events and -1 for background event), according to

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

2160 thus, the reweighting is employed to ensure the minimization of the loss function; a  
 2161 more detailed description of the minimization procedure can be found in Reference  
 2162 [131]. The final classifier output is later used as a final discrimination variable, labeled  
 2163 as *BDT output/response*.

### 2164 5.1.3 Overtraining

2165 Decision trees offer the possibility to have as many nodes as desired in order to  
 2166 reduce the misclassification to zero (in theory); however, when a classifier is too much  
 2167 adjusted to a particular training sample, the classifier's response to a slightly different  
 2168 sample may leads to a completely different classification results; this effect is known  
 2169 as *overtraining*.

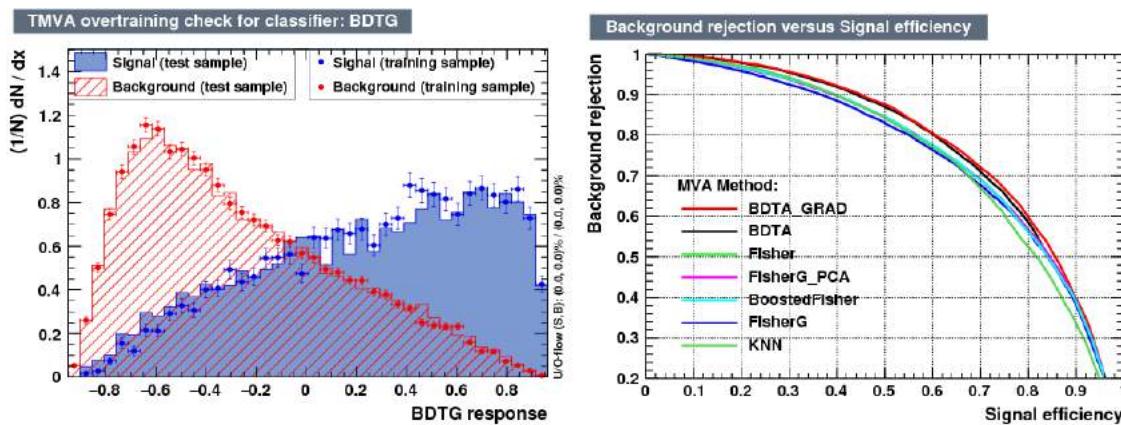
2170 An alternative to reduce the overtraining in BDTs consists in pruning the tree  
 2171 by removing statistically insignificant nodes after the tree growing is completed but  
 2172 this option is not available for BDTs with gradient boosting in the TMVA-toolkit,  
 2173 therefore, the overtraining has to be reduced by tuning the algorithm, number of  
 2174 nodes, minimum number of events in the leaves, etc. The overtraining can be evaluated  
 2175 by comparing the responses of the classifier when running over the training and  
 2176 test samples.

### 2177 5.1.4 Variable ranking

2178 BDTs have a couple of particular advantages related to the input variables; they are  
 2179 relatively insensitive to the number of input variables used in the vector  $\mathbf{x}$ . The  
 2180 ranking of the BDT input variables is determined by counting the number of times a  
 2181 variable is used to split decision tree nodes; in addition, the separation gain-squared  
 2182 achieved in the splitting and the number of events in the node are accounted by  
 2183 applying a weighting to that number. Thus, those variables with small or no power  
 2184 to separate signal and background events are rarely chosen to split the nodes, i.e., are  
 2185 effectively ignored.

2186 In addition, variables correlations play an important role for some MVA methods  
 2187 like the Fisher discriminant algorithm in which the first step consist of performing a  
 2188 linear transformation to a phase space where the correlations between variables are  
 2189 removed; in the case of BDT algorithm, correlations do not affect the performance.

### 2190 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.

2191       The left side of figure 5.5 shows the BDT output distributions for signal ( $pp \rightarrow$   
 2192      $tHq$ ) and background ( $pp \rightarrow t\bar{t}$ ) events; this plot is the equivalent to the one showed  
 2193     in Figure 5.2. A forest with 800 trees, maximum depth per tree = 3, and gradient  
 2194     boosting have been used as training parameters. The BDTG classifier offers a good  
 2195     separation power. There is a small overtraining in the signal distribution, while the  
 2196     background distribution is very well predicted which might indicate that the sample  
 2197     is composed of more background than signal events.

2198       The right side of figure 5.5 shows the background rejection vs signal efficiency  
 2199     curves for several combinations of MVA classifiers-boosting algorithms running over  
 2200     the same MC sample; these curves are known as ROC curves and give an indication  
 2201     of the performance of the classifier. In this particular example, the best performance  
 2202     is achieved with the BDTG classifier (BDTA\_GRAD), which motivate its use in this  
 2203     thesis.

## 2204     **5.2 Statistical inference**

2205       Once events are classified, the next step consists of finding the parameters that define  
 2206     the likelihood functions  $f(\mathbf{x}|s)$ ,  $f(\mathbf{x}|b)$  for signal and background events respectively.  
 2207       In general, likelihood functions depend not only on the measurements but also on  
 2208     parameters ( $\theta_m$ ) that define their shapes; the process of estimating these *unknown*  
 2209     parameters and their uncertainties from the experimental data is called *inference*.

2210       The statistical inference tools used in this analysis are implemented in the RooFit  
 2211     toolkit [132] and COMBINE package [133] included in the CMSSW software frame-  
 2212     work.

2213 **5.2.1 Nuisance parameters**

2214 The unknown parameter vector  $\theta$  is made of two types of parameters: those pa-  
 2215 rameters that provide information about the physical observables of interest for the  
 2216 experiment or *parameters of interest*, and the *nuisance parameters* that are not of  
 2217 a direct interest for the experiment but that need to be included in the analysis in  
 2218 order to achieve a satisfactory description of the data; they represent effects of the  
 2219 detector response like the finite resolutions of the detection systems, miscalibrations,  
 2220 and in general any source of uncertainty introduced in the analysis.

2221 Nuisance parameters can be estimated from experimental data; for instance, data  
 2222 samples from a test beam are usually employed for calibration purposes. In cases  
 2223 where experimental samples are not availables, the estimation of nuisance parameters  
 2224 makes use of dedicated simulation programs to provide the required samples.

2225 The estimation of the unknown parameters involves certain deviations from their  
 2226 true values, hence, the measurement of the nuisance parameter is written in terms  
 2227 of an estimated value, also called central value,  $\hat{\theta}$  and its uncertainty  $\delta\theta$  using the  
 2228 notation

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

2229 where the interval  $[\hat{\theta} - \delta\theta, \hat{\theta} + \delta\theta]$  is called *confidence interval*; it is usually interpreted,  
 2230 in the limit of infinite number of experiments, as the interval where the true value  
 2231 of the unknown parameter  $\theta$  is contained with a probability of 0.6827 (if no other  
 2232 convention is stated); this interval represents the area under a Gaussian distribution  
 2233 in the interval  $\pm 1\sigma$ .

2234 Conventionally, uncertainties are split into two classes: *systematic*, associated with  
 2235 the systematic effects, and *statistical*, related only to fluctuations in data and having

2236 statistical nature.

### 2237 5.2.2 Maximum likelihood estimation method

2238 The estimation of the unknown parameters that are in best agreement with the ob-  
 2239 served data is performed through a function of the data sample that returns the  
 2240 estimate of those parameters; that function is called an *estimator*. Estimators are  
 2241 usually constructed using mathematical expressions encoded in computer programs.

2242 In this thesis, the estimator used is the likelihood function  $f(\mathbf{x}|\boldsymbol{\theta})$ <sup>4</sup> which depends  
 2243 on a set of measured variables  $\mathbf{x}$  and a set of unknown parameters  $\boldsymbol{\theta}$ . The likelihood  
 2244 function for N events in a sample is the combination of all the individual likelihood  
 2245 functions, i.e.,

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

2246 and the estimation method used is the *Maximum Likelihood Estimation* method  
 2247 (MLE); it is based on the combined likelihood function defined by eqn. 5.10 and  
 2248 the procedure seeks for the parameter set that corresponds to the maximum value of  
 2249 the combined likelihood function, i.e., the *maximum likelihood estimator* of the un-  
 2250 known parameter vector  $\boldsymbol{\theta}$  is the function that produces the vector of *best estimators*  
 2251  $\hat{\boldsymbol{\theta}}$  for which the likelihood function  $L(\boldsymbol{\theta})$  evaluated at the measured  $\mathbf{x}$  is maximum.

2252 Usually, the logarithm of the likelihood function is used in numerical algorithm  
 2253 implementations in order to avoid underflow the numerical precision of the computers  
 2254 due to the product of small likelihoods. In addition, it is common to minimize the  
 2255 negative logarithm of the likelihood function, therefore, the negative log-likelihood

---

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

2256 function is

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

2257 The minimization process is performed by the software MINUIT [134] implemented in the ROOT analysis framework. In case of data samples with large number 2258 of measurements, the computational resources necessary to calculate the likelihood 2259 function are too big; therefore, the parameter estimation is performed using binned 2260 distributions of the variables of interest for which the *binned likelihood function* is 2261 given by

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

2263 with  $s_i$  and  $b_i$  the expected number of signal and background yields for the bin  $i$ ,  $n_i$  is 2264 the observed number of events in the bin  $i$  and  $r = \sigma/\sigma_{SM}$  is the signal strength. Note 2265 that the number of entries per bin follows a Poisson distribution. The effect of the 2266 nuisance parameters have been included in the likelihood function through Gaussian 2267 distributions that models the nuisance. The three parameters,  $r$ ,  $s_i$  and  $b_i$  are jointly 2268 fitted to estimate the value of  $r$ .

### 2269 5.3 Upper limits

2270 In this analysis, two hypotheses are considered; the background only hypothesis 2271 ( $H_0(b)$ ) and the signal plus background hypothesis ( $H_1(s+b)$ ), i.e., the sample of 2272 events is composed of background only events ( $r=0$ ) or it is a mixture of signal plus 2273 background events ( $r=1$ ). The exclusion of one hypothesis against the other means 2274 that the observed data sample better agrees with  $H_0$  or rather with  $H_1$ . In order 2275 to discriminate these hypotheses, a test statistic is constructed on the basis of the

2276 likelihood function evaluated for each of the hypothesis.

2277 The *Neyman-Pearson* lemma [135] states that the test statistic that provides the  
 2278 maximum power for  $H_1$  for a given significance level (background misidentification  
 2279 probability  $\alpha$ ), is given by the ratio of the likelihood functions  $L(\mathbf{x}|H_1)$  and  $L(\mathbf{x}|H_0)$ ;  
 2280 however, in order to use that definition it is necessary to know the true likelihood  
 2281 functions, which in practice is not always possible. Approximate functions obtained  
 2282 by numerical methods, like the BDT method described above, have to be used, so  
 2283 that the *profile likelihood* test statistic is defined by

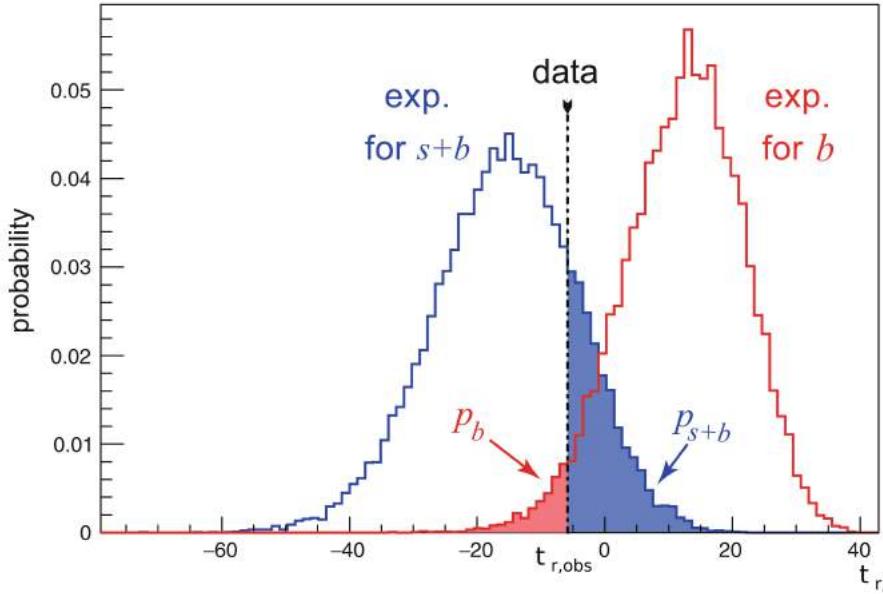
$$\lambda(\mathbf{r}) = \frac{L(\mathbf{x}|r, \hat{\boldsymbol{\theta}}(r))}{L(\mathbf{x}|\hat{r}, \hat{\boldsymbol{\theta}})}, \quad (5.13)$$

2284 where,  $\hat{r}$  and  $\hat{\boldsymbol{\theta}}$  maximize the likelihood function, and  $\hat{\boldsymbol{\theta}}$  maximizes the likelihood  
 2285 function for a given value of the signal strength modifier  $r$ . In practice, the test  
 2286 statistic  $t_r$

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

2287 is used to evaluate the presence of signal in the sample, since the minimum of  $t_r$  at  
 2288  $r = \hat{r}$  suggests the presence of signal with signal strength  $\hat{r}$ . The uncertainty interval  
 2289 for  $r$  is determined by the values of  $r$  for which  $t_r = +1$ .

2290 The expected probability density function (p.d.f)  $f(t_r|r, \boldsymbol{\theta})$  of the test statistic  $t_r$   
 2291 can be obtained numerically by generating MC samples where one hypothesis,  $H_0(b)$   
 2292 or  $H_1(s+b)$ , is assumed; thus, MC samples contain the possible values of  $t_r$  obtained  
 2293 from *pseudo-experiments* as shown in Figure 5.6. The probability that  $t_r$  takes a value  
 2294 equal or greater than the observed value ( $t_{r,obs}$ ) when a signal with a signal modifier  
 2295  $r$  is present in the data sample, is called the *p-value* of the observation; it can be  
 2296 calculated using



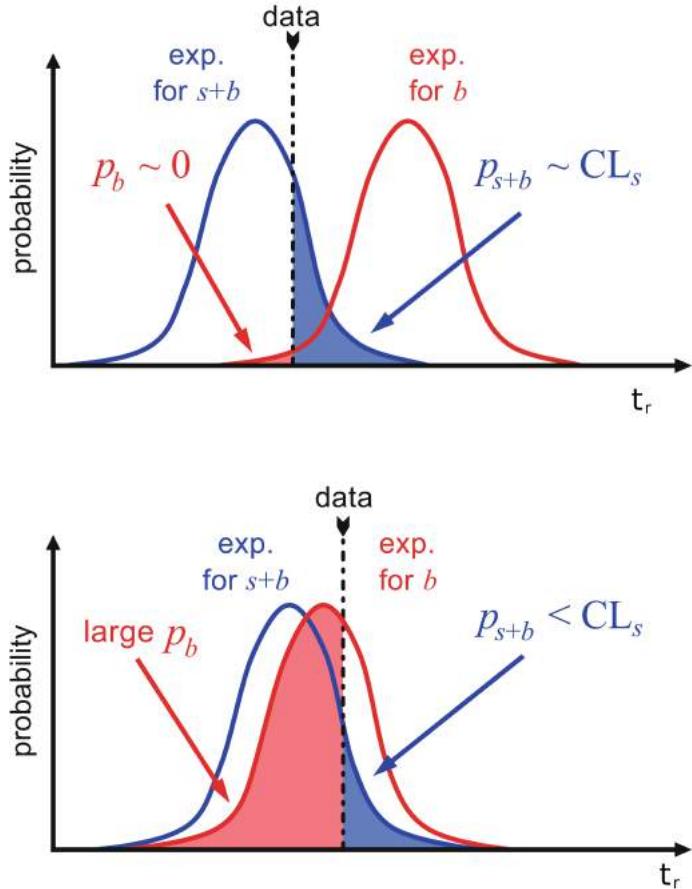
**Figure 5.6:**  $t_r$  p.d.f. from MC pseudo experiments assuming  $H_0$  (red) and  $H_1$  (blue). The black dashed line shows the value of the test statistic as measured from data. Adapted from Reference [128].

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

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



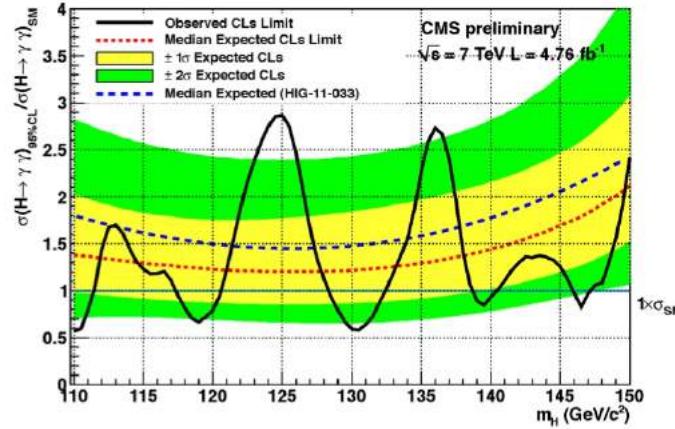
**Figure 5.7:**  $CL_s$  limit illustration. When the test statistic p.d.f. for the two hypotheses  $H_0$  and  $H_1$  are well separated (top) and when they are largely overlapped (bottom). Adapted from Reference [128].

2305 background-only hypothesis. These issues are corrected by using the modified p-  
2306 value [136]

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

2307 If  $H_1$  is true, then  $p_b$  is small,  $CL_s \simeq p_r$  and  $H_0$  is rejected; if there is large  
2308 overlap and a statistical fluctuation causes that  $p_b$  is large, then both numerator and  
2309 denominator in Eqn. 5.17 become small but  $CL_s$  would allow the rejection of  $H_1$   
2310 even if there is poor sensitivity to signal.

2311        The upper limit of the parameter of interest  $r^{up}$  is determined by excluding the  
 2312   range of values of  $r$  for which  $CL_s(r, \theta)$  is lower than the confidence level desired,  
 2313   normally 90% or 95%, e.g, scanning over  $r$  and finding the value for which  $p_r'^{up} =$   
 2314   0.05. The expected upper limit can be calculated using pseudo-experiments based on  
 2315   the background-only hypothesis and obtaining a distribution for  $r_{ps}^{up}$ ; the median of  
 2316   that distribution corresponds to the expected upper limit, while the  $\pm 1\sigma$  and  $\pm 2\sigma$   
 2317   deviations correspond to the values of the distribution that defines the 68% and 95%  
 2318   of the area under the distribution centered in the median. It is usual to present all  
 2319   the information about the expected and observed limits in the so-called *Brazilian-flag*  
 2320   *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].

## 2321        5.4 Asymptotic limits

2322   As said before, the complexity of the likelihood functions, the construction of test  
 2323   statistics, and the calculation of the limits and their uncertainties is not always man-  
 2324   ageable and requires extensive computational resources; in order to overcome those  
 2325   issues, asymptotic approximations for likelihood-based test statistics, like the ones

2326 described in previous sections, have been developed [138, 139] using Wilks' theorem.  
2327 Asymptotic approximations replace the construction of the test statistics p.d.f.s using  
2328 MC pseudo-experiments, with the approximate calculation of the test statistics p.d.f.s  
2329 by employing the so-called *Asimov dataset*.

2330 The Asimov dataset is defined as the dataset that produce the true values of the  
2331 nuisance parameters when it is used to evaluate the estimators for all the parameters;  
2332 it is obtained by setting the values of the variables in the dataset to their expected  
2333 values [139].

2334 Limits calculated by using the asymptotic approximation and the Asimov dataset  
2335 are know as *asymptotic limits*.

<sup>2336</sup> **Chapter 6**

<sup>2337</sup> **Search for production of a Higgs**

<sup>2338</sup> **boson and a single top quark in**

<sup>2339</sup> **multilepton final states in pp**

<sup>2340</sup> **collisions at  $\sqrt{s} = 13$  TeV**

<sup>2341</sup> **6.1 Introduction**

<sup>2342</sup> The Higgs boson discovery, supported on experimental observations and theoretical  
<sup>2343</sup> predictions made about the SM, gives the clue of the way in that elementary parti-  
<sup>2344</sup> cles acquire mass through the Higgs mechanism; therefore, knowing the Higgs mass,  
<sup>2345</sup> the Higgs-vector boson and Higgs-fermion couplings can be tested. In order to test  
<sup>2346</sup> the Higgs-top coupling, several measurements have been performed, as stated in the  
<sup>2347</sup> chapter 1, but they are limited in sensitivity to measure the square of the coupling.  
<sup>2348</sup> The production of a Higgs boson in association with a single top quark ( $tH$ ) not  
<sup>2349</sup> only offers access to the sign of the coupling, but also, to the CP phase of the Higgs

2350 couplings.

2351 This chapter presents the search for the associated production of a Higgs boson  
 2352 and a single top quark ( $tHq$ ) events, focusing on leptonic signatures provided by the  
 2353 Higgs decay modes to  $WW$ ,  $ZZ$ , and  $\tau\tau$ ; the 13 TeV dataset produced in 2016, with  
 2354 an integrated luminosity of  $35.9\text{fb}^{-1}$ , is used.

2355 As shown in Section 1.5, the SM cross section of  $tHq$  process is affected by a  
 2356 destructive interference between two contributions (see Figure 1.15), where the Higgs  
 2357 couples to either the W boson or the top quark; however, if the sign of the Higgs-  
 2358 top coupling is flipped with respect to the SM prediction, a large enhancement of  
 2359 the cross section occurs, making this analysis sensitive to such deviation. A second  
 2360 process, where the Higgs boson and top quark are accompanied by a W boson ( $tHW$ )  
 2361 has similar behavior, albeit with a weaker interference pattern and lower contribution  
 2362 to the cross section, therefore, a combination of both processes would increase the  
 2363 sensitivity to the sign of the coupling; in this analysis both contributions are combined  
 2364 and referred to as  $tH$  channel. A third contribution comes from  $t\bar{t}H$  process. The  
 2365 purpose of this analysis is to investigate the exclusion of the presence of the  $tH +$   
 2366  $t\bar{t}H$  processes in the SM under the assumption of the anomalous Higgs-top coupling  
 2367 modifier ( $\kappa_t = -1$ ). The analysis exploits signatures with two leptons of the same sign  
 2368 ( $2lss$ ) channel and three leptons ( $3l$ ) channel in the final state.

2369 Constraints on the sign of the Higgs-top coupling ( $y_t$ ) have been derived from the  
 2370 decay rate of Higgs boson to photon pairs [50] and from the cross section for associated  
 2371 production of Higgs and Z bosons via gluon fusion [141], with recent results disfavoring  
 2372 negative signs of the coupling [44, 59, 142], although the negative sign coupling have  
 2373 not been completely excluded.

2374 The analysis presented here, expands previous analyses performed at 8 TeV [143,  
 2375 144] and searches for associated production of  $t\bar{t}$  pair and a Higgs boson in the mul-

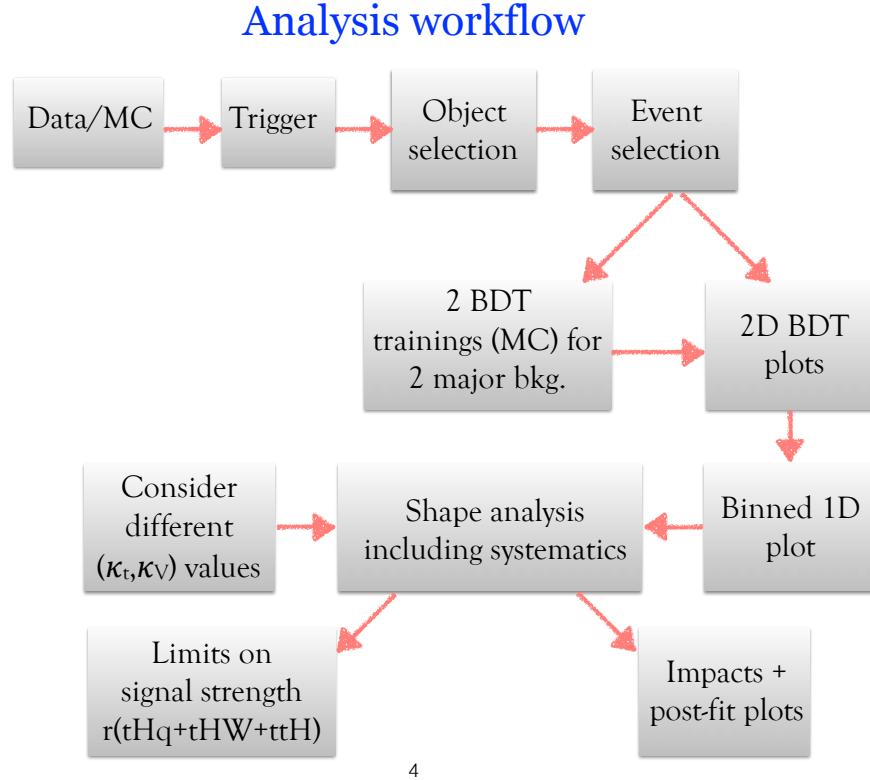
2376 tilepton final state channel [145]; it also complements searches in  $H \rightarrow b\bar{b}$  [146].

2377 The first sections present the characteristic  $tHq$  signature as well as the expected  
 2378 backgrounds. The MC samples, data sets, and the physics object definitions are then  
 2379 described; after, the background predictions, the signal extraction, the statistical  
 2380 treatment of the selected events and the discussion of the systematic uncertainties  
 2381 are described. The final section presents the results for the exclusion limits as a  
 2382 function of the ratio of  $\kappa_t$  and the dimensionless modifier of the Higgs-vector boson  
 2383 coupling  $\kappa_V$ .

2384 The analysis is designed to efficiently identify and select prompt leptons from on-  
 2385 shell W and Z boson decays and to reject non-prompt leptons from  $b$  quark decays  
 2386 and spurious lepton signatures from hadronic jets. Events are then selected in the  
 2387  $2lss$  and  $3l$  channels, and are required to contain hadronic jets, some of which must  
 2388 be consistent with  $b$  quark hadronization. Finally, the signal yield is extracted by  
 2389 simultaneously fitting the output of two dedicated multivariate discriminants, trained  
 2390 to separate the  $tHq$  signal from the two dominant backgrounds, in all categories. The  
 2391 fit result is then used to set an upper limit on the combined  $t\bar{t}H + tH$  production  
 2392 cross section, as a function of the relative coupling strengths of Higgs-top quark and  
 2393 Higgs-Vector boson. Figure 6.1 shows an schematic overview of the analysis strategy  
 2394 workflow.

2395 With respect to the 8 TeV analysis, the object selections have been adjusted for  
 2396 the updated LHC running conditions at 13 TeV, the lepton identification has been  
 2397 improved, and more powerful multivariate analysis techniques are used for the signal  
 2398 extraction.

2399 The analysis has been made public by CMS as a Physics Analysis Summary [147]  
 2400 combining the result for the three lepton and two lepton same-sign channels; the  
 2401 content present in this chapter is based on that document and on References [145,149]

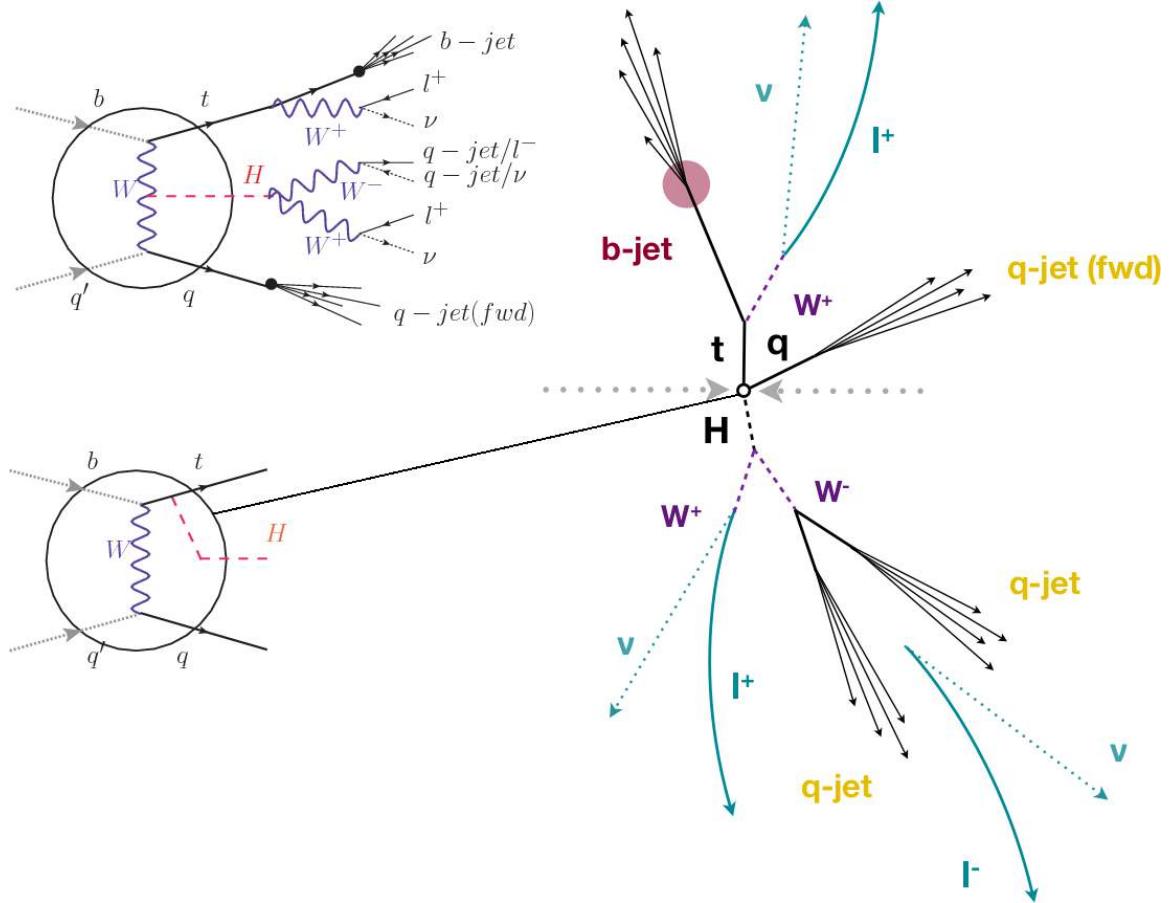


**Figure 6.1:** A schematic overview of the analysis workflow. Based on sets of optimized physics object definitions and selection criteria, signal and background events in a data sample are discriminated. The discrimination is performed by a BDT, previously trained using MC samples of the dominant backgrounds, 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.

2407  $tHq$  process from the  $pp$  collision to the final state configuration. A single top quark  
 2408 is produced accompanied by a light quark, denoted as  $q$ ; this light quark is produced  
 2409 predominantly in the forward region of the detector. The Higgs boson can be either  
 2410 emitted by the exchanged  $W$  boson or directly by the singly produced top quark.

2411 Due to their high masses/short lifetimes, top quark and Higgs boson decay after  
 2412 their production within the detector. The Higgs boson is required to decay into a  $W$

2413 boson pair<sup>1</sup>. The top quark almost always decays into a bottom quark and a W boson,  
 2414 as encoded in the CMK matrix. The W bosons are required to decay leptonically  
 2415 either all the three in the  $3l$  channel or the pair with equal electrical charge in the  
 2416  $2lss$  channel case;  $\tau$  leptons are not reconstructed separately and only their leptonic  
 2417 decays into either electrons or muons are considered in this analysis.

2418 In summary, the signal process is characterized by a the final state with

- 2419 • one light-flavored forward jet,
  - 2420 • one central b-jet,
  - 2421 •  $2lss$  channel → two leptons of the same sign, two neutrinos and two light (often  
 2422 soft) jets,
  - 2423 •  $3l$  channel → three leptons, three neutrinos and no central light-flavored jets,
- 2424 The presence of neutrinos is inferred from the presence of MET.

## 2425 6.3 Background processes

2426 The background processes are those that can mimic the signal signature or at least  
 2427 can be reconstructed as signal as a result of certain circumstances. The backgrounds  
 2428 can be classified as

- 2429 • irreducible backgrounds: where genuine prompt leptons are produced in on-  
 2430 shell W and Z boson decays; they can be reliably estimated directly from MC  
 2431 simulated events, using higher-order cross sections or data control regions for  
 2432 the overall normalization.

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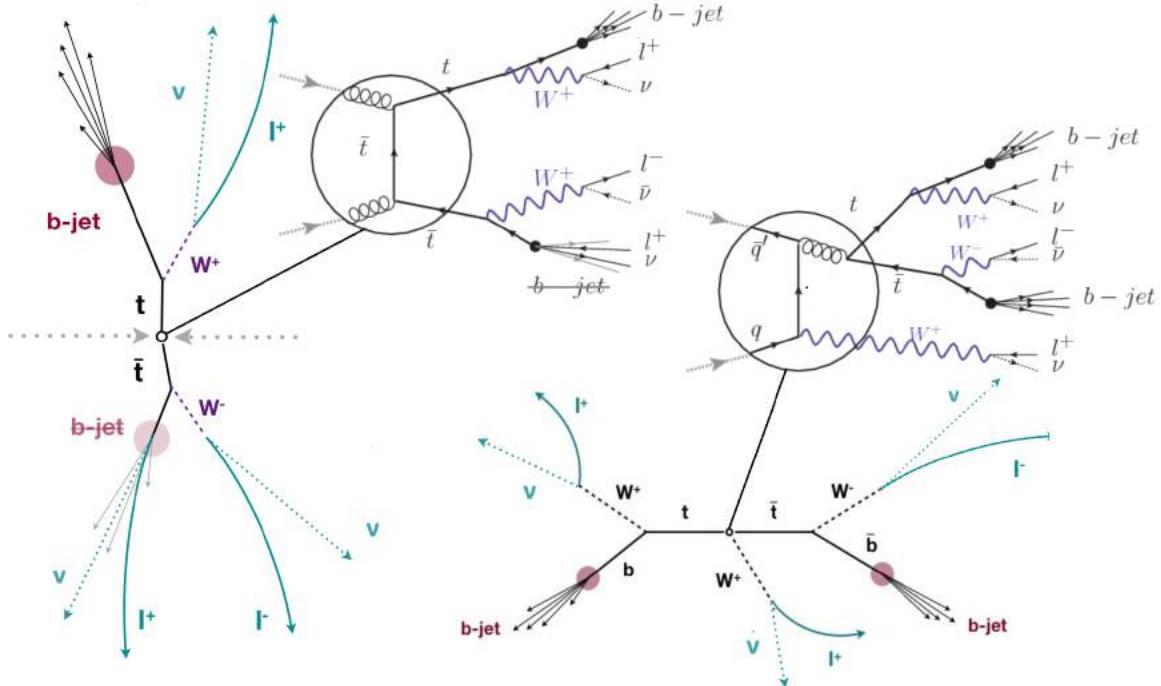
<sup>1</sup> ZZ and  $\tau\tau$  decays are also include in the analysis but they are not separately reconstructed

2433     • reducible backgrounds: where at least one of the leptons is *non-prompt*, i.e.,  
 2434       produced within a hadronic jet; genuine leptons from heavy flavor decays and  
 2435       misreconstructed jets, also known as *mis-ID leptons* are considered non-prompt  
 2436       leptons or or *fake leptons* as well as electrons from photon conversions. These  
 2437       non-prompt leptons leave tracks and hits in the detection systems as would a  
 2438       prompt lepton, but evaluation the correlation of those hits with nearby jets  
 2439       could be a way of removing them. The misassignment of electron charge in  
 2440       processes like  $t\bar{t}$  or Drell-Yan, represents an additional source of background,  
 2441       but it is relevant only for the  $2lss$  channel. Reducible backgrounds are not well  
 2442       predicted by simulation, hence, they are estimated using data-driven methods.

2443       The main sources of background events for  $tHq$  process are  $t\bar{t}$  process and  $t\bar{t}V(V =$   
 2444        $W, Z, \gamma$ ) processes. Figure 6.3 shows the signature for  $t\bar{t}$  and  $t\bar{t}W$  processes.

2445       The largest contribution to irreducible backgrounds comes from  $t\bar{t}W$  and  $t\bar{t}Z$   
 2446       processes for which the number of ( $b-$ )jets (( $b-$ )jet multiplicity) is higher than that  
 2447       of the signal events, while for other contributing background events,  $WZ$ ,  $ZZ$ , and  
 2448       rare SM processes like  $W^\pm W^\pm qq$ ,  $t\bar{t}t\bar{t}$ ,  $tZq$ ,  $tZW$ ,  $WWW$ ,  $WWZ$ ,  $WZZ$ ,  $ZZZ$ ,  
 2449       the ( $b-$ )jet multiplicity is lower compared to that of the signal events. None of the  
 2450       irreducible backgrounds present activity in the forward region of the detector.

2451       On the side of the reducible backgrounds, the largest contribution comes from the  
 2452        $t\bar{t}$  events which have a very similar signature to the signal events but does no present  
 2453       activity in the forward region of the detector either; A particular feature of the  $t\bar{t}$   
 2454       events is their charge-symmetry, which is different from the characteristics of signal  
 2455       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.

## 2456 6.4 Data and MC Samples

### 2457 6.4.1 Full 2016 data set

2458 The data set used in this analysis was collected by the CMS experiment during 2016,  
 2459 while running at  $\sqrt{s} = 13$  TeV, and corresponds to a total integrated luminosity  
 2460 of  $35.9 \text{ fb}^{-1}$ . Only periods when the CMS magnet was on were considered when  
 2461 selecting the data samples; that corresponds to the 23Sep2016 (Run B to G) and  
 2462 PromptReco (Run H) versions of the datasets.

2463 Multilepton final states with either two same-sign leptons or three leptons tar-  
 2464 get the case where the Higgs boson decays to a pair of  $W$  bosons,  $\tau$  leptons, or  $Z$   
 2465 bosons, and where the top quark decays leptonically, hence, the SingleElectron,

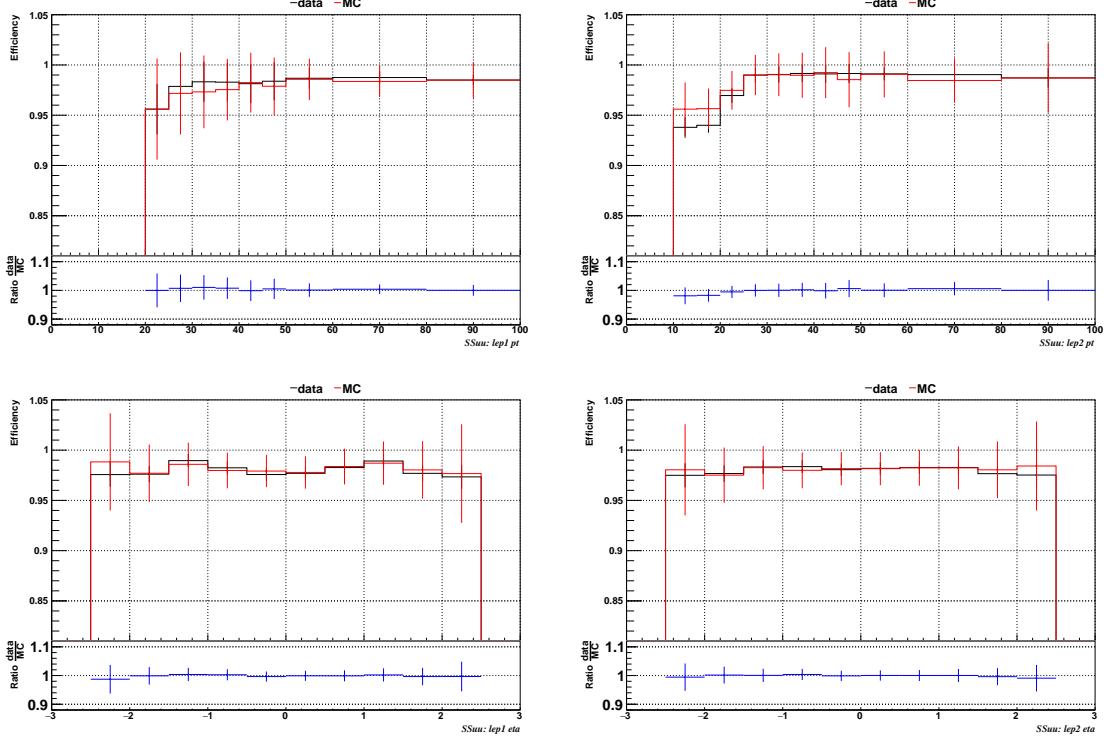
2466 SingleMuon, DoubleEG, MuonEG, DoubleMuon dataset (see Table A.1) compose the  
 2467 full dataset. The certified luminosity sections are selected using the golden JSON file  
 2468 defined by the CMS experiment [148].

## 2469 6.4.2 Triggers

2470 The events considered are those online-reconstructed events triggered by one, two, or  
 2471 three leptons. Single-lepton triggers are included in order to boost the acceptance  
 2472 of events where the  $p_T$  of the sub-leading lepton falls below the threshold of the  
 2473 double-lepton triggers. The trigger efficiency is increased by including double-lepton  
 2474 triggers in the  $3l$  category, and single-lepton triggers in all categories; it is possible  
 2475 given the logical “or” of the trigger decisions of all the individual triggers in a given  
 2476 category. Table A.2 shows the lowest-threshold non-prescaled triggers present in the  
 2477 High-Level Trigger (HLT) menus for both Monte-Carlo and data in 2016.

## 2478 Trigger efficiency scale factors

2479 Trigger efficiency describes the ability of events to pass the trigger requirements. It  
 2480 is measured in simulated events using generator information given that there is no  
 2481 trigger bias with the MC sample. Measuring the trigger efficiency in data requires a  
 2482 more elaborated procedure; first, select a set of events collected by a trigger that is  
 2483 uncorrelated with the lepton triggers such that the selected events form an unbiased  
 2484 sample. In this analysis, that uncorrelated trigger is a MET trigger. Second step  
 2485 is looking for candidate events with exactly two good leptons (exactly three good  
 2486 leptons for the  $3l$  channel). Finally, measure the efficiency for the candidate events to  
 2487 pass the logical “or” of triggers being considered in a given event category as defined  
 2488 in Table A.2.

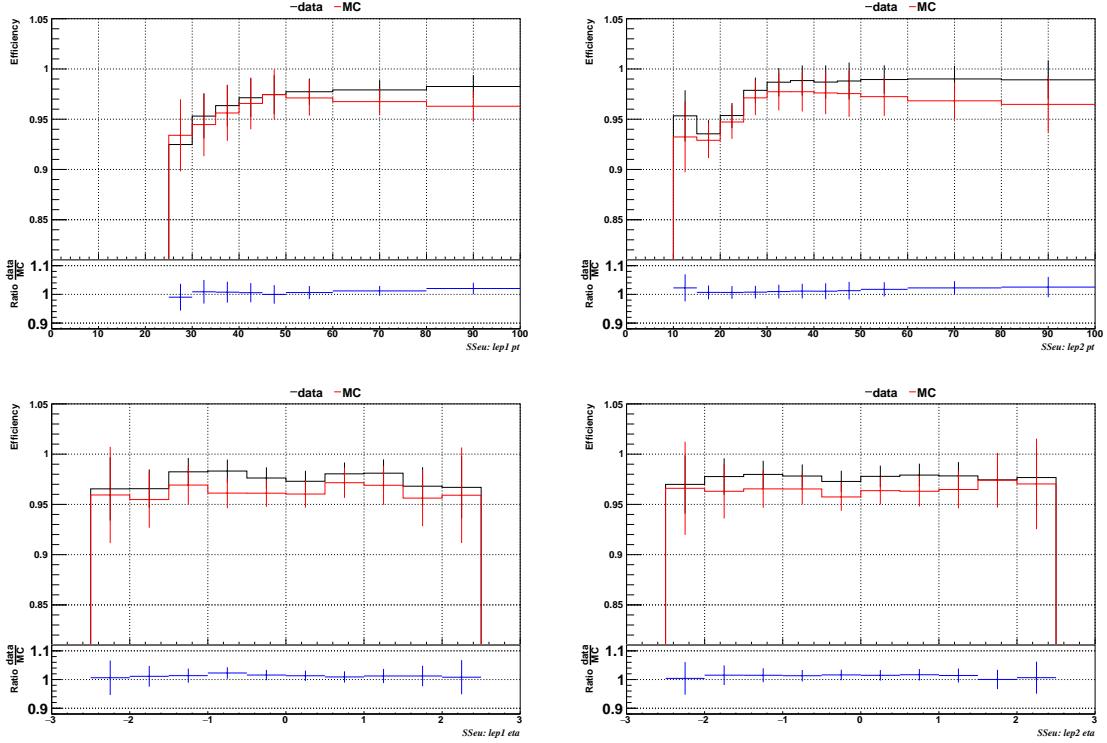


**Figure 6.4:** Comparison between data and MC trigger efficiencies in the same-sign  $\mu\mu$  category, as a function of the  $p_T$  (top) and  $\eta$  (bottom) of the leading lepton (left) and the sub-leading lepton (right) [149].

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.

2489 Comparisons between the data and MC efficiencies for each category, showed in  
 2490 Figures 6.4, 6.5, and 6.6, reveal that they are in good agreement; the difference is  
 2491 corrected by applying scale factors derived from the ratio between both efficiencies.  
 2492 Applied flat scale factors in each category are shown in Table 6.1; they have been  
 2493 inherited from Reference [149].

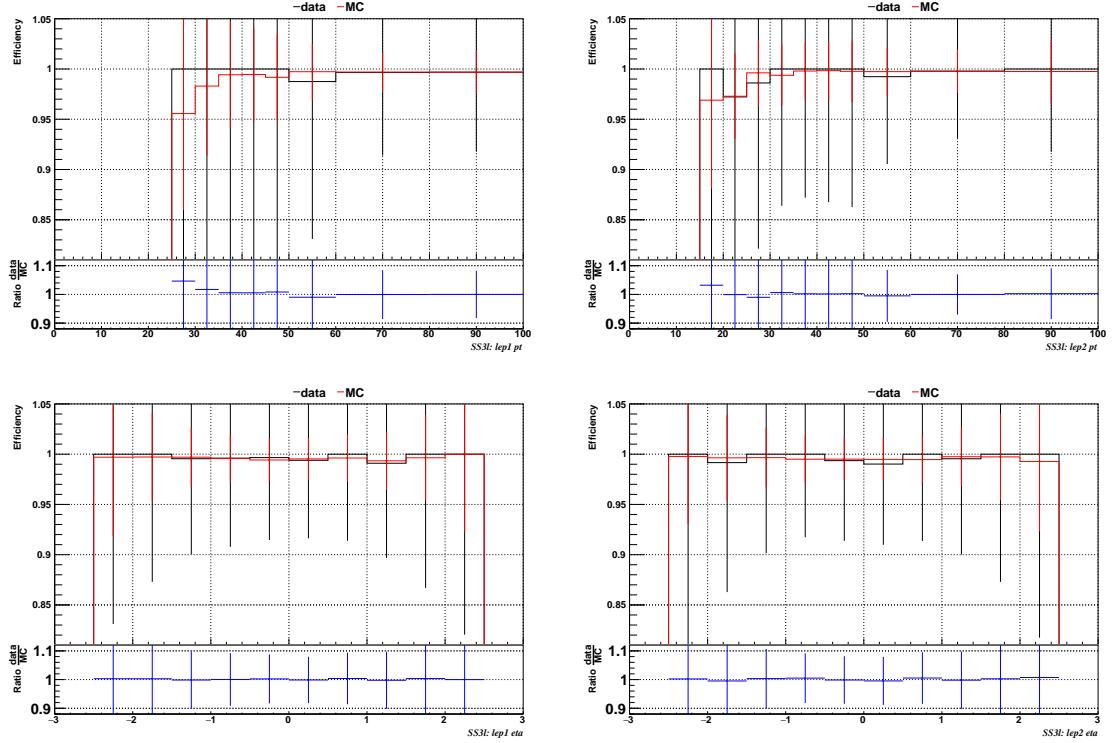


**Figure 6.5:** Comparison between data and MC trigger efficiencies in the same-sign  $e\mu$  category as a function of the  $p_T$  (top) and  $\eta$  (bottom) of the leading lepton (left) and the sub-leading lepton (right) [149].

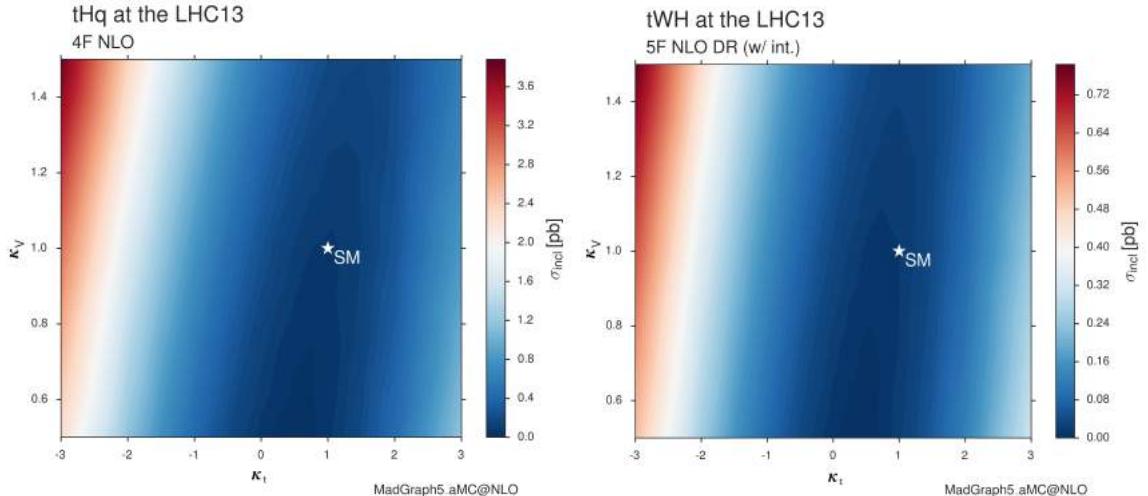
### 2494 6.4.3 MC samples

2495 Current event generators allow the adjustment of the kinematics of the generated  
 2496 events, based on an event-wise reweighting; in this way, several generation parameters  
 2497 phase spaces can be explored according to the experimental interests. The signal  
 2498 samples used in this analysis were generated in such a way that not only the case  $\kappa_t$   
 2499  $= -1$ , but an extended range of  $\kappa_t$  and  $\kappa_V$  values may be investigated.

2500  $tHq$  and  $tHW$  cross section in the  $\kappa_t$ - $\kappa_V$  phase space are shown in Figure 6.7. As  
 2501 said in section 3.1, the  $tHq$  sample was generated using the 4F scheme which provides  
 2502 a better description of the additional  $b$  quark from the initial gluon splitting, while the  
 2503  $tHW$  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].

2504 with  $t\bar{t}H$  at LO.

2505 **MC signal samples**

2506 The two signal samples,  $tHq$  and  $tHW$ , correspond to the `RunIISummer16MiniAODv2`  
 2507 campaign produced with `CMSW_80X`; they were produced with `MG5_aMC@NLO`  
 2508 (version 5.2.2.3), in LO mode at  $\sqrt{s} = 13$  TeV, and are normalized to NLO cross sec-  
 2509 tions (see Table 6.2). The Higgs boson is assumed to be SM-like except for the values  
 2510 of its couplings to the top quark and W boson. Each sample was generated with a set  
 2511 of event weights corresponding to 51 different values of  $(\kappa_t, \kappa_V)$  couplings, accessible  
 2512 in terms of LHE event weights as shown in Table A.3; however, the main interest is  
 2513 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

2514 **Table 6.2:** MC signal samples used in this analysis; cross section and branching fraction  
 2515 are also listed [150].

2514 The  $t\bar{t}H$  sample was produced using `AMC@NLO` interfaced to `PYTHIA 8` for  
 2515 the parton shower, and is scaled to NLO cross sections. The  $t\bar{t}H$  cross section depends  
 2516 quadratically on  $\kappa_t$ ; however, in contrast to the  $tHq$  and  $tHW$  samples, the scaling  
 2517 is not performed during the sample generation process but in the analysis code since  
 2518 it was decided to include the  $t\bar{t}H$  process as a part of the signal in the course of the  
 2519 analysis.

2520 **MC background samples**

2521 Several MC generators were used to generate the samples of the background processes.  
 2522 The dominant background sources ( $t\bar{t}$ ,  $t\bar{t}W$ ,  $t\bar{t}Z$ ) were produced using `AMC@NLO`

2523 interfaced to PYTHIA8, and are scaled to NLO cross sections. Other minor back-  
 2524 ground processes are simulated using POWHEG interfaced to PYTHIA, or bare  
 2525 PYTHIA as stated in the sample names in Table A.4. Pileup interactions are in-  
 2526 cluded in the simulation in order to reflect the observed multiplicity in data; the  
 2527 simulated events are weighted according to the actual pileup in data, estimated from  
 2528 the measured bunch-to-bunch instantaneous luminosity and the total inelastic cross  
 2529 section, 69.2 mb. All events are finally passed through a full simulation of the CMS  
 2530 detector using GEANT4, and reconstructed using the same algorithms as used for  
 2531 the data.

## 2532 **6.5 Object Identification**

2533 In this section, the specific definitions of the physical objects in terms of the recon-  
 2534 struction parameters are presented; thus, the provided details summarize and com-  
 2535 plement the descriptions presented in previous chapters. The object reconstruction  
 2536 and selection strategy used in this thesis are inherited from the analyses in Refer-  
 2537 ences [145, 149].

### 2538 **6.5.1 Lepton reconstruction and identification**

2539 Two types of leptons are defined in this analysis: *signal leptons* are those coming from  
 2540  $W, Z$  and  $\tau$  decays which usually are isolated from other particles; *background leptons*  
 2541 are defined as leptons produced in  $b$ -jet hadron decays, light-jets misidentification,  
 2542 and photon conversions.

2543 The process of reconstruction and identification of electron and muon candidates  
 2544 was described in chapter 3, hence, the identification variables used in order to retain

2545 the highest possible efficiency for signal leptons while maximizing the rejection of  
 2546 background leptons are listed and described in the following sections <sup>2</sup>.

2547 The identification variables include not only observables related directly to the re-  
 2548 constructed leptons themselves, but also to the clustered energy deposits and charged  
 2549 particles in a cone around the lepton direction (jet-related variables); an initial loose  
 2550 preselection of leptons candidates is performed and then an MVA discriminator, re-  
 2551 fered to as *lepton MVA* discriminator, is used to distinguish signal leptons from  
 2552 background leptons.

## 2553 Muons

2554 The Physics Objects Groups (POG) at CMS, are in charge of studying and defining  
 2555 the set of selection criteria applied on the course of reconstruction and identification  
 2556 of particles. These selection criteria are implemented in the CMS framework in the  
 2557 form of several object identification working points according to the strength of the  
 2558 requirements.

2559 The muon candidates are reconstructed by combining information from the tracker  
 2560 system and the muon detection system of CMS detector and the POG defined three  
 2561 working points for muon identification *MuonID* [153];

- 2562     • *POG Loose Muon ID* is a particle identified as a muon by the PF event re-  
     2563 construction and also reconstructed either as a global-muon or as an arbitrated  
     2564 tracker-muon. This identification criteria is designed to be highly efficient for  
     2565 prompt muons and for muons from heavy and light quark decays; it can be com-  
     2566 plemented by applying impact parameter cuts in analyses with prompt muon  
     2567 signals.

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

- 2568     • *POG Medium Muon ID* is a Loose muon with additional track-quality and  
 2569       muon-quality (spatial matching between the individual measurements in the  
 2570       tracker and the muon system) requirements. This identification criteria is de-  
 2571       signed to be highly efficient in the separation of the muons coming from decay  
 2572       in flight of heavy quarks and muons coming from B meson decays as well as  
 2573       prompt muons. An additional category *MVA Prompt ID* is defined in this iden-  
 2574       tification criteria directed to discriminated muons from B mesons and prompt  
 2575       muons (from W,Z and  $\tau$  decays). The Medium ID provides the same fake rate as  
 2576       the Tight Muon ID but a higher efficiency on prompt and B-decays muons. [154]  
  
 2577     • *POG Tight Muon ID* is a global muon with additional muon-quality require-  
 2578       ments Tight Muon ID selects a subset of the PF muons.

2579       Only muons within the muon system acceptance  $|\eta| < 2.4$  and minimum  $p_T$  of 5  
 2580       GeV are considered.

## 2581     **Electrons**

2582       Electrons are reconstructed using information from the tracker and from the electro-  
 2583       magnetic calorimeter and identified by an MVA algorithm (*MVA eID* discriminant)  
 2584       using the shape of the calorimetric shower variables like the shape in  $\eta$  and  $\phi$ , the clus-  
 2585       ter circularity, widths along  $\eta$  and  $\phi$ ; track-cluster matching variables like  $E_{tot}/p_{in}$ ,  
 2586        $E_{Ele}/p_{out}$ ,  $\Delta\eta_{in}$ ,  $\Delta\eta_{out}$ ,  $\Delta\phi_{in}$ ,  $1/E - 1/p$ ; and track quality variables like  $\chi^2$  of the  
 2587       GSF tracks, the number of hits used by the GSF filter [155].

2588       A loose selection based on  $\eta$ -dependent cuts on this discriminant is used to prese-  
 2589       lect electron candidates, the full shape of the discriminant is used in the lepton MVA  
 2590       selection to separate signal leptons from background leptons (described in Section  
 2591       6.5.1).

2592 In order to reject electrons from photon conversions, electron candidates with  
 2593 missing hits in the pixel tracker layers or matched to a conversion secondary vertex  
 2594 are discarded. Electrons are selected for the analysis if they have  $p_T > 7$  GeV and  
 2595 are located within the tracker system acceptance region ( $|\eta| < 2.5$ ).

2596 **Lepton vertexing and pile-up rejection**

2597 The impact parameter in the transverse plane  $d_0$ , impact parameter along the  $z$ -  
 2598 axis  $d_z$ , and the impact parameter significance in the detector space  $SIP_{3D}$ , are  
 2599 considered to perform the identification and rejection of pile-up, misreconstructed  
 2600 tracks, and background leptons from b-hadron decays; pile-up and misreconstructed  
 2601 track mitigation is achieved by imposing loose cuts on the impact parameter variables.  
 2602 The full shape of those variables is used in a lepton MVA classifier to achieve the best  
 2603 separation between the signal and the background leptons.

2604 **Lepton isolation**

2605 PF is able to recognize leptons from two different sources: on one side, leptons from  
 2606 the decays of heavy particles, such as W and Z bosons, which are normally isolated in  
 2607 space from the hadronic activity in the event; on the other side, leptons from decays  
 2608 of hadrons and jets misidentified as leptons, which are not isolated as the former. For  
 2609 highly boosted systems, like the lepton and the  $b$ -jet generated in the semileptonic  
 2610 decay of a boosted top, the decay products tend to be more closer and sometimes they  
 2611 even overlap; thus, the PF standard definition of isolation in terms of the separation  
 2612  $\Delta R$  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.

2627 **Jet-related variables**

2628 In order to reject misidentified leptons from  $b$ -jets, mostly coming from  $t\bar{t}$ +jets,  
 2629 Drell-Yan+jets, and W+jets events, the vertexing and isolation described in previous  
 2630 sections are complemented with additional variables related to the closest recon-  
 2631 structed jet to the lepton, i.e., the PF jets reconstructed<sup>3</sup> around the leptons with  
 2632  $\Delta R = \sqrt{(\eta^l - \eta^{jet})^2 + (\phi^l - \phi^{jet})^2} < 0.5$ . The identification variables used in the lep-  
 2633 ton MVA discriminator are the ratio  $p_T^l/p_T^{jet}$ , the CSV b-tagging discriminator value  
 2634 of the jet, the number of charged tracks of the jet, and the relative  $p_T$  given by

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

2635 **LeptonMVA discriminator**

2636 Electrons and muons passing the basic selection process described above are referred  
 2637 to as *loose leptons*. Additional discrimination between signal leptons and background  
 2638 leptons is crucial considering that the rate of  $t\bar{t}$  production is much larger than the  
 2639 signal, hence, an overwhelming background from  $t\bar{t}$  production is present. To maxi-  
 2640 mally exploit the available information in each event to that end, the dedicated lepton  
 2641 MVA discriminator, based on a boosted decision tree (BDT) algorithm, has been built  
 2642 so that all the identification variables can be used together.

2643 The lepton MVA discriminator training is performed using simulated signal Loose  
 2644 leptons from the  $t\bar{t}H$  MC sample and fake leptons from the  $t\bar{t}$  +jets MC sample,  
 2645 separately for muons and electrons. The input variables used include vertexing, iso-  
 2646 lation and jet-related variables, the  $p_T$  and  $\eta$  of the lepton, the electron MVA eID  
 2647 discriminator and the muon segment-compatibility variables. An additional require-  
 2648 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  $\Delta R > 0.4$ .

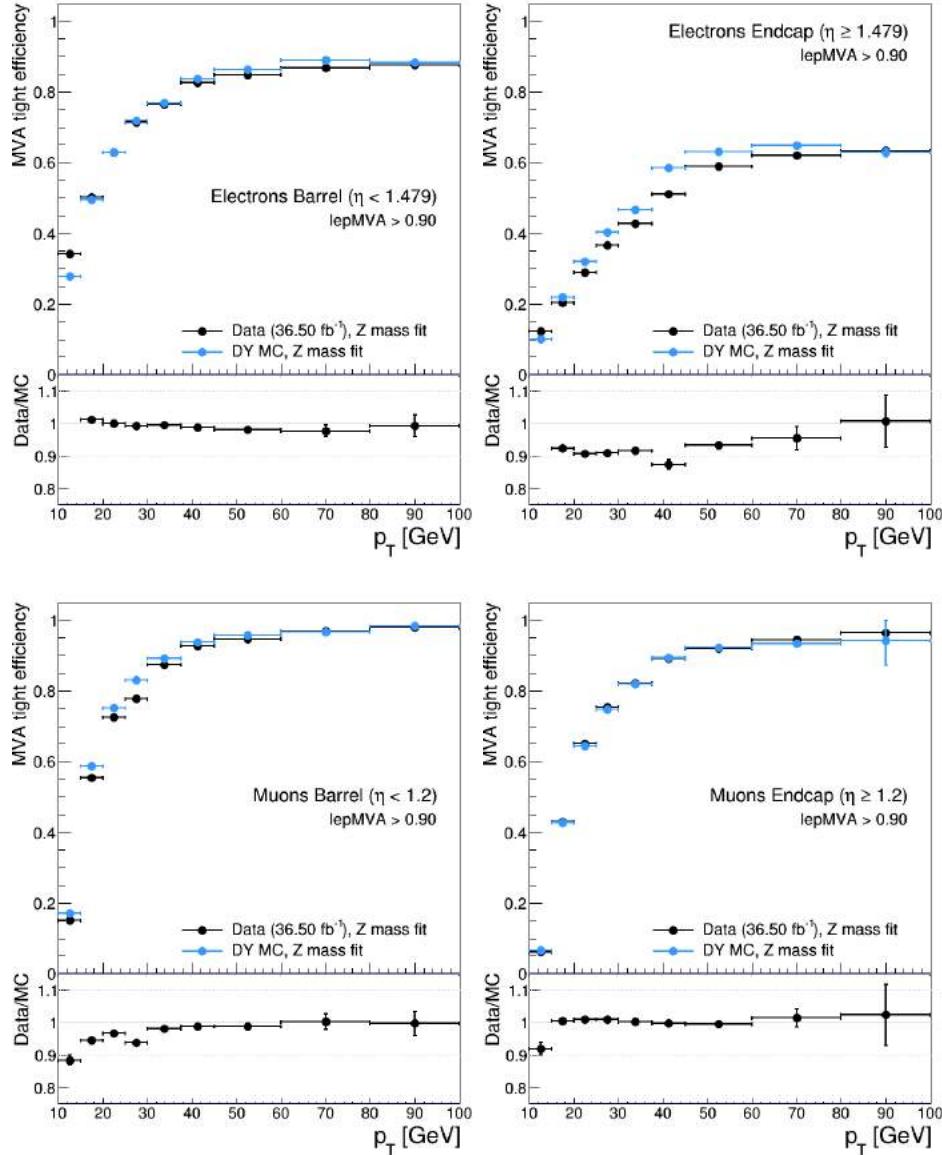
Cut	Loose	Fakeable object	Tight
$ \eta  < 2.4$	✓	✓	✓
$p_T$	$> 5\text{GeV}$	$> 15\text{GeV}$	$> 15\text{GeV}$
$ d_{xy}  < 0.05 \text{ (cm)}$	✓	✓	✓
$ d_z  < 0.1 \text{ (cm)}$	✓	✓	✓
$\text{SIP}_{3D} < 8$	✓	✓	✓
$I_{\text{mini}} < 0.4$	✓	✓	✓
is Loose Muon	✓	✓	✓
jet CSV	—	$< 0.8484$	$< 0.8484$
is Medium Muon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

2674 **6.5.2 Lepton selection efficiency**



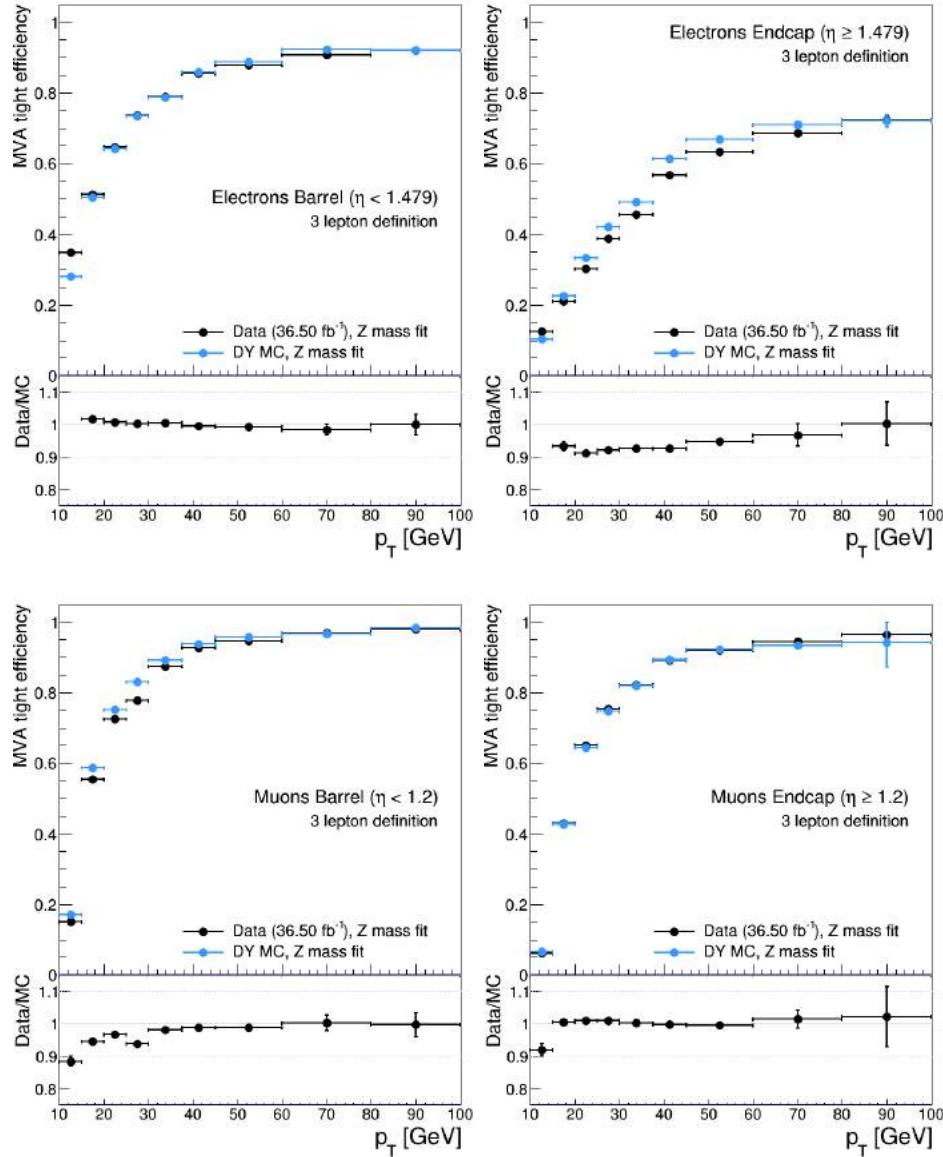
**Figure 6.8:** Tight vs loose selection efficiencies for electrons (top), and muons (bottom), for the  $2lss$  definition, i.e., including the tight-charge requirement.

2675        Efficiencies of reconstruction and selecting loose leptons are measured both for  
 2676        muons and electrons using a tag and probe method on both data and MC, using  
 2677         $Z \rightarrow \ell^+ \ell^-$  [157]. The scale factors are derived from the ratio of efficiencies  $\varepsilon_i(p_T, \eta)$

2678 measured for a given lepton in data/MC, according to

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

2679 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.

2680 full sample; therefore, the full simulation correction is given by the product of all  
 2681 the individual scale factors. The scale factors used in this thesis are inherited from  
 2682 Reference [149] which in turns inherited them from leptonic SUSY analyses using  
 2683 equivalent lepton selections.

2684 The efficiency of applying the tight selection as defined in Tables 6.4 and 6.5, on  
 2685 the loose leptons is determined by using a tag and probe method on a sample of Drell-  
 2686 Yan enriched events. Figures 6.8 and 6.9 show the efficiencies for the  $2lss$  channel and  
 2687  $3l$  channel respectively. Efficiencies in the  $2lss$  channel have been produced including  
 2688 the tight-charge requirement, while for the  $3l$  channel it is not included. Number  
 2689 of passed and failed probes are determined from a fit to the invariant mass of the  
 2690 dilepton system. Simulation is corrected using these scale factors; note that they  
 2691 depend on  $\eta$  and  $p_T$ .

### 2692 **6.5.3 Jets and $b$ -jet tagging**

2693 In this analysis, jets are reconstructed by clustering PF candidates using the anti- $k_t$   
 2694 algorithm with parameter distance  $\Delta R = 0.4$ ; those charged hadrons that are not  
 2695 consistent with the selected primary vertex are discarded from the clustering. The  
 2696 jet energy is then corrected for the varying response of the detector as a function of  
 2697 transverse momentum  $p_T$  and pseudorapidity  $\eta$ . Jets are selected for being used in the  
 2698 analysis only if they have  $p_T > 25$  GeV and are separated from any selected leptons  
 2699 by  $\Delta R > 0.4$ .

2700 Jets coming from the primary vertex and jets coming from pile-up vertices are  
 2701 distinguished using a MVA discriminator based on the differences in the jet shapes,  
 2702 in the relative multiplicity of charged and neutral components, and in the different  
 2703 fraction of transverse momentum which is carried by the most energetic components.

2704 Jet tracks are also required to be compatible with the primary vertex.

2705 Jets originated from the hadronization of a  $b$  quark are selected using a MVA  
 2706 likelihood discriminant which uses track-based lifetime information and reconstructed  
 2707 secondary vertices (CSV algorithm). Only jets within the CMS tracker acceptance  
 2708 ( $\eta < 2.4$ ) are identified with this tool. Data samples are used to measure the efficiency  
 2709 of the  $b$ -jet tagging and the probability to misidentify jets from light quarks or gluons;  
 2710 in both cases the measurements are parametrized as a function of the jet  $p_T$  and  $\eta$   
 2711 and later used to correct differences between the data and MC simulation in the  $b$   
 2712 tagging performance, by applying per-jet weights to the simulation, dependent on  
 2713 the jet  $p_T$ ,  $\eta$ ,  $b$  tagging discriminator, and flavor (from the MC generation/simulation  
 2714 truth information) [151]. The per-event weight is taken as the product of the per-jet  
 2715 weights, including those of the jets associated to the leptons. The weights are derived  
 2716 on  $t\bar{t}$  and Z+jets events.

2717 Two working points are defined, based on the CSV algorithm output: *loose* work-  
 2718 ing point ( $\text{CSV} > 0.46$ ) with a  $b$  signal tagging efficiency of about 83%, and *medium*  
 2719 working point ( $\text{CSV} > 0.80$ ) with  $b$ -tagging efficiency of about 69% [152]. Tagging of  
 2720 jets from charm quarks have efficiencies of about 40% and 18% for loose and medium  
 2721 working points respectively. Separate scale factors are applied to jets originating from  
 2722 bottom/charm quarks and from light quarks in simulated events to match the tagging  
 2723 efficiencies measured in the data.

#### 2724 6.5.4 Missing Energy MET

2725 As stated in Section 3.4.1, the MET vector is calculated as the negative of the vector  
 2726 sum of transverse momenta of all PF candidates in the event and its magnitude is  
 2727 referred to as  $E_T^{\text{miss}}$ . Due to pile-up interactions, the performance in determining

2728 MET is degraded; in order to correct for that, the energy from the selected jets and  
 2729 leptons that compose the event is assigned to the variable  $H_T^{miss}$ . It is calculated in  
 2730 the same way as  $E_T^{miss}$  and although it has worse resolution than  $E_T^{miss}$ , it is more  
 2731 robust in the sense that it does not rely on the soft part of the event. The event  
 2732 selection uses a linear discriminator based on the two variables given by

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

2733 taking advantage of the fact that the correlation between  $E_T^{miss}$  and  $H_T^{miss}$  is less  
 2734 for events with instrumental missing energy than for events with real missing energy.  
 2735 The working point  $E_T^{miss, LD} > 0.2$  was chosen to ensure a good signal efficiency while  
 2736 keeping an efficient background rejection.

## 2737 6.6 Event selection

2738 Events are selected considering the features of the signal process and the decay sig-  
 2739 nature as described in Section 6.2. At the trigger level, events are selected to contain  
 2740 either one, two, or three leptons with minimal  $p_T$  thresholds:

- 2741 • single-lepton trigger → 24 GeV for muons and at 27 GeV for electrons
- 2742 • double-lepton triggers → leading and sub-leading leptons: 17 and 8 GeV for  
 2743 muons and 23 and 12 GeV for electrons.
- 2744 • three-lepton triggers → threshold on the third hardest lepton in the event: 5  
 2745 and 9 GeV for muons and electrons, respectively.

2746 The offline event selection level targets the specific topology of the  $tHq$  signal  
 2747 with  $H \rightarrow WW$  and  $t \rightarrow Wb \rightarrow l\nu b$ ; therefore, the resulting state is composed of three

2748 W bosons, one  $b$  quark, and a light spectator quark at high rapidity. The selection  
 2749 criteria for the two channels exploited in this analysis are summarized in Table 6.6.  
 2750 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 $\rightarrow p_T > 40\text{ GeV}, \eta > 2.4$
$E_{T,LD}^{miss} > 0.2$	
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.

2751 In the  $2lss$  channel, events with additional tight leptons are vetoed as well as those  
 2752 for which a loose lepton pair has an invariant mass below 12 GeV. A threshold in  $p_T$  of  
 2753 the leading and sub-leading leptons is also required. Events where the two electrons  
 2754 have invariant mass within 10 GeV of the Z boson mass ( $Z$ -veto) are discarded in  
 2755 order to reject events from DY+jets production with charge misidentified electrons.  
 2756 In addition, contribution from the associated production of two W bosons of equal  
 2757 charge and two light jets  $W^\pm W^\pm qq$  and from same-sign W boson pairs can also be  
 2758 produced in double parton scattering (DPS) processes, where each of the colliding  
 2759 protons gives two partons, resulting in two hard interactions.

2760 In the  $3l$  lepton channel, leptons are required to have respectively  $p_T > 25\text{GeV}, >$   
 2761  $> 15\text{ GeV}$ , and  $> 15\text{ GeV}$ . Events with an opposite-sign same-flavor lepton combination  
 2762 (OSSF) with invariant mass within 15 GeV of the Z boson mass are discarded in order  
 2763 to reject events from  $WZ + \text{jets}$  production.

## 2764 6.7 Background modeling and predictions

2765 The dominant background contribution is expected to arise from top quark produc-  
2766 tion processes, either  $t\bar{t}$  pair production or in  $t\bar{t}$  associated production with a W/Z.  
2767 Processes with production of single top quarks also contribute, mainly in the associ-  
2768 ated production with a Z boson ( $tZq$ ) or when produced with both a W and a Z boson  
2769 ( $tZW$ ). Background contamination from diboson processes is strongly suppressed by  
2770 imposing the Z-veto, vetoing additional leptons and requiring  $b$ -jets in the event.

2771 The selection criteria in Table 6.6 represent a relatively loose selection that allows  
2772 to maintain a large signal efficiency while suppressing the main backgrounds; thus  
2773 that selection is called *pre-selection*. The events obtained from the pre-selection are  
2774 then used to extract the signal contribution in a second analysis step, using BDT dis-  
2775 criminators against the main backgrounds of  $t\bar{t}W/t\bar{t}Z$  and non-prompt leptons from  
2776  $t\bar{t}$ . The shape of the discriminator variables is then fit to the observed data distribu-  
2777 tion to estimate the signal and background yields, simultaneously for all channels.

2778 Irreducible backgrounds are reliably estimated from MC simulated events; there-  
2779 fore, in this analysis all backgrounds involving prompt leptons are estimated in this  
2780 way. Reducible backgrounds, like non-prompt lepton backgrounds, are not well pre-  
2781 dicted by simulation, hence, they are estimated using data-driven methods.

### 2782 6.7.1 $t\bar{t}V$ and diboson backgrounds

2783 Backgrounds from  $t\bar{t}W$  and  $t\bar{t}Z$  processes are estimated using simulated events, cor-  
2784 rected for data/MC differences and inefficiencies (trigger and lepton selection) in the  
2785 same way as signal events. Their production cross sections are calculated at NLO of  
2786 QCD and EWK, considering theoretical uncertainties from unknown higher orders of  
2787 12% for  $t\bar{t}W$  and 10% for  $t\bar{t}Z$ . Additional uncertainties arise from the knowledge of

2788 PDFs and  $\alpha_s$  of about 4% each for  $t\bar{t}W$  and  $t\bar{t}Z$ .

2789 The diboson contribution is also estimated from simulated events; however, the  
 2790 overall normalization of this process is obtained from a dedicated control region.  
 2791 The motivation behind that strategy is that even though the measured inclusive  
 2792 cross section for diboson processes ( $WZ, ZZ$ ) is in good agreement with the NLO  
 2793 calculations [149], that agreement is perturbed when leptonic  $Z$  decays and hadronic  
 2794 jets in the final state are required; those requirements are precisely the ones that  
 2795 make the diboson production a background for the  $tHq$  signal. Thus, by using a  
 2796 dedicated control region dominated by  $WZ$  production<sup>4</sup>, the overall normalization is  
 2797 constrained.

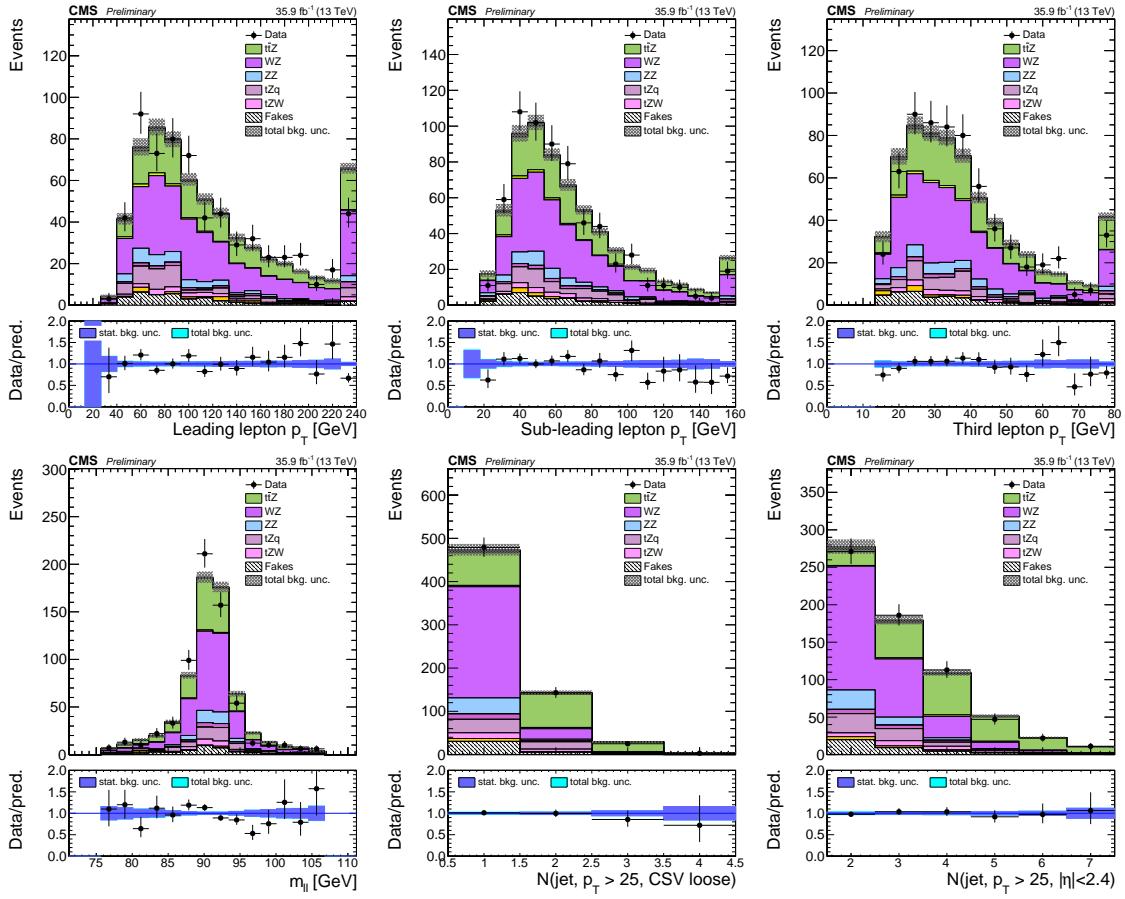
2798 The control region is defined by the presence of at least three leptons, of which  
 2799 one opposite-sign pair must be compatible with a  $Z$  boson decay, i.e., invert the  $Z$ -  
 2800 veto which makes the control region orthogonal to signal region; the b-jet tagging  
 2801 requirements is also inverted with respect to the signal region, i.e., require two not  
 2802  $b$ -jets. A scale factor is extracted from the predicted distribution of  $WZ$  events in the  
 2803 control region, and the observed data, while keeping other processes fixed; this factor  
 2804 is used to scale the diboson prediction in the signal selection region. More details  
 2805 about the procedure used can be found in Reference [149] from where the scale factor  
 2806 is taken.

2807 In order to test the usability of the diboson background scale factor in this analysis,  
 2808 a  $Z$ -enriched control region<sup>5</sup> was defined by inverting the  $Z$ -veto and requiring exactly  
 2809 three tight leptons with  $p_T > 25/15/15$  GeV, one or more jets passing the CSVv2 loose  
 2810 working point and less than four central jets. Figure 6.10 shows the distribution of  
 2811 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.

2812 data motivates the adoption of the diboson background scale factor.

2813 Most of the diboson events passing the signal selection contain jets from light  
 2814 quarks and gluons that are incorrectly tagged as  $b$ -jets; it makes the estimate mainly  
 2815 sensitive to the experimental uncertainty in the mis-tag rate rather than the theore-  
 2816 tical uncertainty in the jet flavor composition. The overall uncertainty assigned to  
 2817 the diboson prediction is estimated from the statistical uncertainty due to the limited  
 2818 sample size in the control region (30%), the residual background in the control region  
 2819 (20%), the uncertainties on the  $b$ -tagging rate (10-40%), and from the knowledge of  
 2820 PDFs and the theoretical uncertainties of the extrapolation (up to 10%).

2821 **6.7.2 Non-prompt and charge mis-ID backgrounds**

2822 The non-prompt lepton background contribution to the final selection is estimated  
 2823 using the fake factor method. The main idea of the method is to define a control  
 2824 region of events enriched in the background to estimate and determine a factor that  
 2825 relates (extrapolates) these events to those in the signal region. The method is data-  
 2826 driven in the sense that the control sample is selected from data, and the extrapolation  
 2827 factor is measured from data.

2828 In the signal region of this analysis, non-prompt leptons are predominantly pro-  
 2829 duced in  $t\bar{t}$  events, with a much smaller contribution, from Drell-Yan production;  
 2830 therefore, the control region also known as *application region*, is defined by modifying  
 2831 the event selection criteria in such a way that most of the events after selection are  
 2832  $t\bar{t}$  events and thus the misidentification rate is increased. The application regions  
 2833 for electrons and muons are defined by the *fakeable* object definitions in Tables 6.4  
 2834 and 6.5. Since the *fakeable* definition is a loosened version of the tight definition, in  
 2835 the context of fake rates, the *fakeable* definition becomes the loose selection.

2836 The ratio between the number of events that pass both, the loose and tight se-  
 2837 lections, and the number of events that pass the loose selection but fail the tight  
 2838 one, corresponds to the *loose-to-tight ratio or fake factor/rate (f)*. The measurement  
 2839 of the fake factor is made using two background dominated data samples, collected  
 2840 with dedicated triggers, as a function of  $p_T$  and  $|\eta|$  and separately for muons and  
 2841 electrons:

- 2842     • A sample dominated by QCD multijet events, collected using single lepton trig-  
 2843       gers at relatively high  $p_T$  thresholds. It is used to extract ratios for lepton  
 2844       candidates with  $p_T$  above 30 GeV.
- 2845     • A sample dominated by Z + jets events, where the two high  $p_T$  leptons resulting

2846 from the Z decay are used to trigger the events without biasing the  $p_T$  spectrum  
 2847 of a third lepton at low transverse momentum. It is used to determine the ratios  
 2848 for low  $p_T$  leptons.

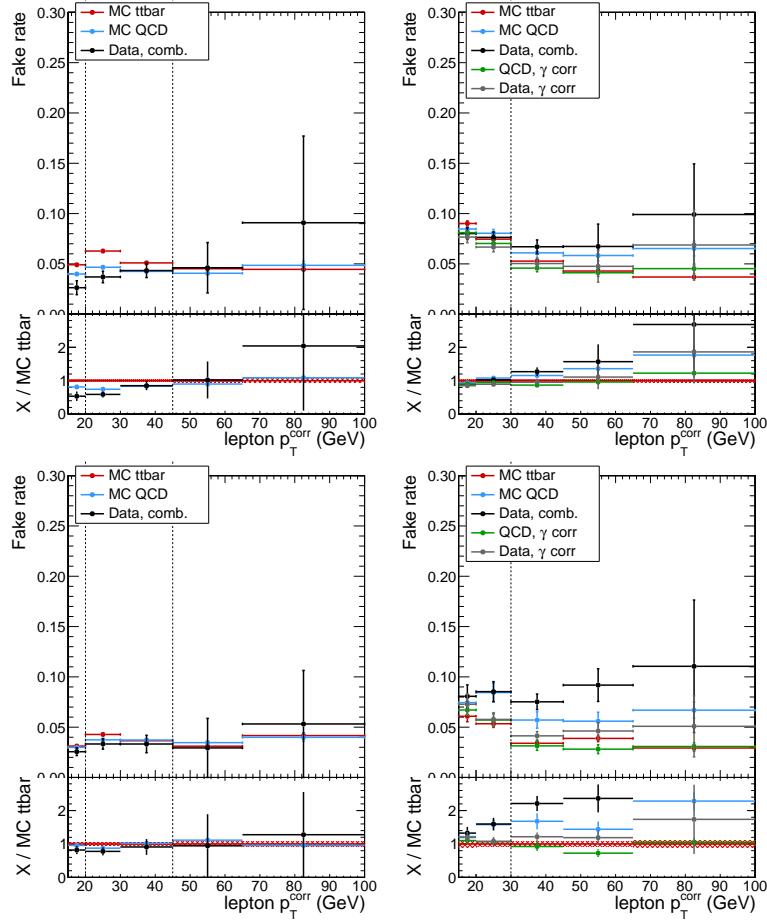
2849 Processes like  $W + \text{jets}$ ,  $Z + \text{jets}$ ,  $WZ$  and  $ZZ$  produce prompt leptons that  
 2850 contaminate the samples; thus, they are suppressed by vetoing additional leptons in  
 2851 the selection, and the residual contamination is then subtracted using the transverse  
 2852 mass as a discriminating variable.

2853 The extrapolation from the application region to the signal region is performed  
 2854 by weighting the events in the application region using the fake factor according to  
 2855 the following rules:

- 2856 • events with one lepton failing the tight criteria are weighted with the factor  
 2857  $\frac{f}{(1-f)}$  for the estimate to the signal region.
- 2858 • events with two leptons (i,j) failing the tight criteria are weighted with the factor  
 2859  $-\frac{f_i f_j}{(1-f_i)(1-f_j)}$  for the estimate to the signal region.
- 2860 • events with three leptons (i,j,k) failing the tight criteria are weighted with the  
 2861 factor  $\frac{f_i f_j f_k}{(1-f_i)(1-f_j)(1-f_k)}$  for the estimate to the signal region.

2862 Figure 6.11 shows the fake rates for electrons and muons used in this analysis  
 2863 which were taken from the studies in Reference [149].

2864 The resulting prediction of the event yield in the signal selection carries an uncer-  
 2865 tainty of 30-50% which is composed of the statistical uncertainty in the measurement  
 2866 of the fake rates due to prescaling of lepton triggers, the uncertainty in the subtraction  
 2867 of residual prompt leptons from the control region, and from testing the closure of the  
 2868 method in simulated background events; hence, it is one of the dominant limitations  
 2869 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.

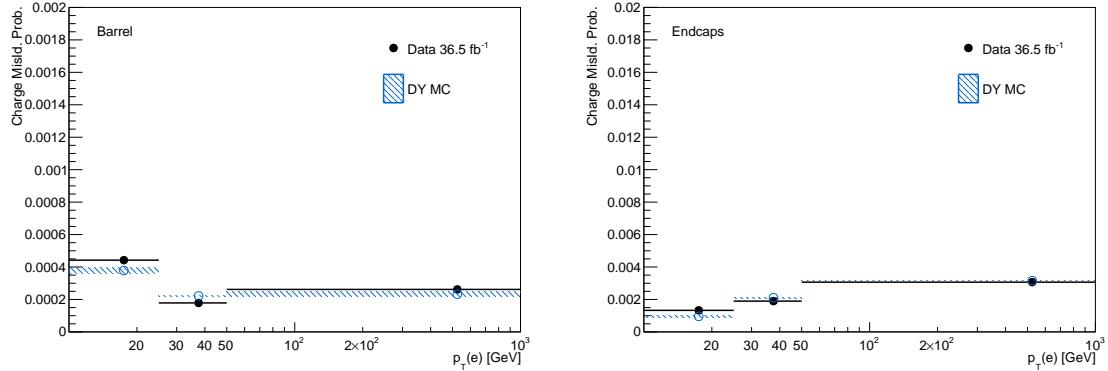
The charge mis-ID background is estimated from the yield of opposite-sign event in the signal region by measuring the charge mis-ID probability in same-sign and opposite-sign events compatible with a Z boson decay, in several bins of  $p_T$  and  $\eta$ ,

2878 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].

2879 The charge mis-ID probability is found to be negligible for this analysis for muons,  
 2880 whereas for electrons it ranges from about 0.02% in the barrel section ( $|\eta| < 1.48$ )  
 2881 up to about 0.35% in the detector endcaps ( $1.48 < |\eta| < 2.5$ ). as shown in Table 6.7  
 2882 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].

2883 The contribution from charge mis-ID electrons in signal selection of this analysis  
 2884 comes mainly from  $t\bar{t}$  and Drell-Yan events. The systematic uncertainty of the nor-  
 2885 malization of the charge mis-ID estimate is evaluated at about 30%, arising from a  
 2886 slight disagreement of the mis-ID probability between data and simulation. Given  
 2887 that it only affects the  $e\mu$  channel, its impact on the final sensitivity is very limited.

## 2888 6.8 Pre-selection yields

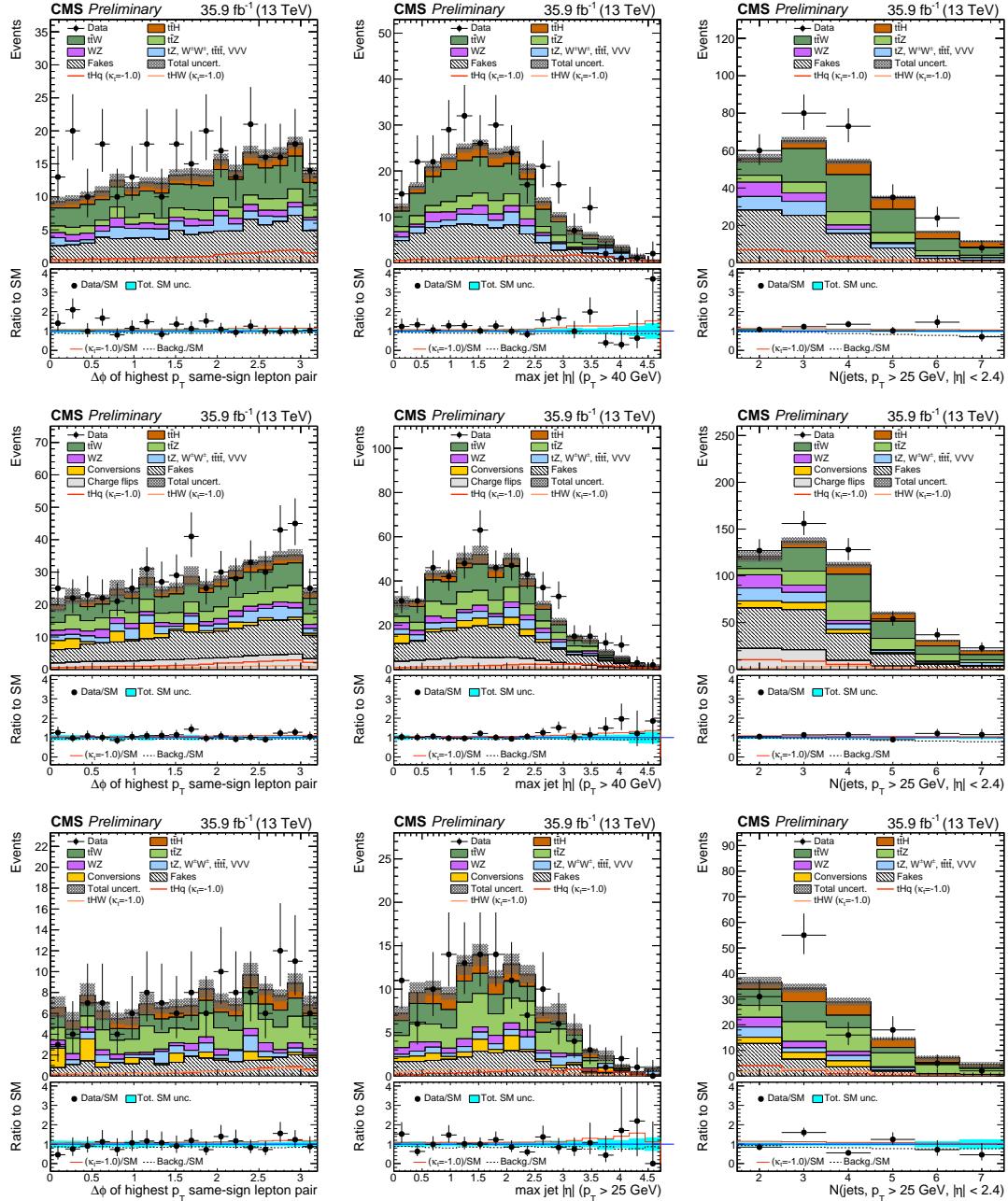
2889 The expected and observed event yields of the pre-selection are shown in Table 6.8;  
 2890 Figure 6.13 shows the distributions of some relevant kinematic variables, normalized  
 2891 to the cross section of the respective processes and to the integrated luminosity. The  
 2892 remaining variables 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.

2893 For the  $tH$  and  $t\bar{t}H$  processes, the largest contribution comes from Higgs decays  
 2894 to WW (about 75%), followed by  $\tau\tau$  (about 20%) and ZZ (about 5%). Other Higgs  
 2895 production modes contribute negligible event yields (< 5% of the  $tH + t\bar{t}H$  yield) as  
 2896 shown in Table 6.9.

2897 A significant fraction of selected data events (about 50% in the dilepton channels,  
 2898 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.

2899 search for  $t\bar{t}H$  in multilepton channels [149]. This is particularly important when  
 2900 considering a possible combination of the measurements from both studies. More  
 2901 details about the overlap between these two analyses are presented in Appendix E.

## 2902 6.9 Signal discrimination

2903 The production cross section for the signal processes  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  is only  
 2904 about 600 fb (the enhancement provided by inverted couplings,  $\kappa_t = -1$  almost double  
 2905 it), resulting in a small signal to background ratio even for a tight selection. A  
 2906 multivariate method is hence employed to train discriminators to separate  $tH$  signal  
 2907 events from the dominant background events.

2908 **6.9.1 MVA classifiers evaluation**

2909 Several MVA classifier algorithms were evaluated in order to determine the most  
 2910 appropriate method for this analysis<sup>6</sup>. The comparison is based on the performance  
 2911 of the classifiers, encoded in the plot of the background rejection as a function of the  
 2912 signal efficiency (ROC curve). The top row of Figure 6.14 shows the ROC curves for  
 2913 evaluated methods; two separated training were performed in the  $3l$  channel: against  
 2914  $t\bar{t}$  (right) and  $t\bar{t}V$  (left) processes.

2915 In both cases, the gradient boosted decision tree *BDTG* (*BDTA\_GRAD* in the  
 2916 plot) classifier offers the best results, followed by the adaptive BDT classifier (*BDTA*);  
 2917 the several Fisher classifiers tested, which differ in their parameters and/or boosting  
 2918 method, they offer similar performance among them, while the k-Nearest Neighbour  
 2919 (kNN) classifier performance is below the rest of the classifiers. The corresponding  
 2920 ROC curves and in the  $2lss$  channel for trainings against  $t\bar{t}V$ (left) and  $t\bar{t}$  (right)  
 2921 processes are shown in the bottom row of Figure 6.14; the BDTG performance is  
 2922 similar to that in the  $3l$  channel.

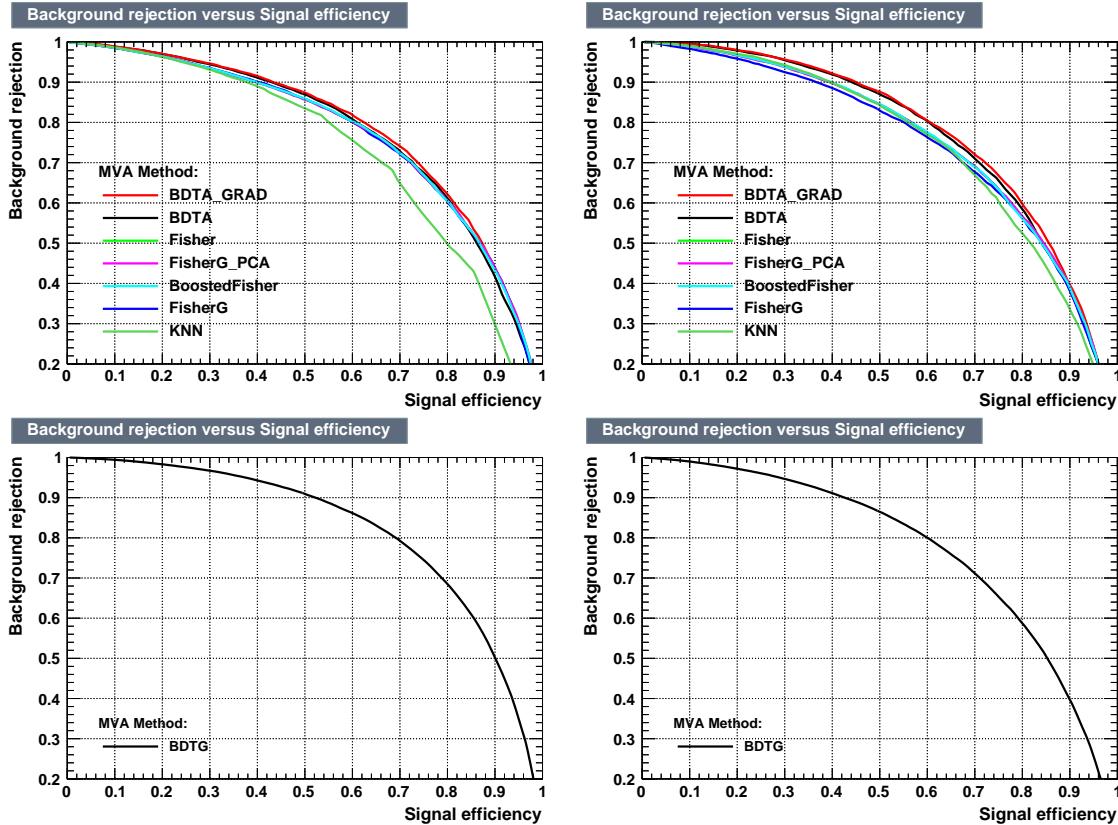
2923 **6.9.2 Discriminating variables**

2924 The classifier chosen to separate the  $tHq$  signal from the main backgrounds is the  
 2925 *BDTG* classifier, trained on simulated signal and background events. The samples  
 2926 used in the training are the  $tHq$  sample in Table 6.2, the samples in the third section  
 2927 of Table A.4 and the samples marked with an \* in the same table.

2928 As explained in Section 5.1.1, a set of discriminating variables are given as input to  
 2929 the *BDTG* which combines the individual discrimination power of each input variable

---

<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  $t\bar{V}$  (left) and  $t\bar{t}$  (right). Bottom: background rejection vs signal efficiency (ROC curve) in the  $2lss$  channel for a single discriminator: BDTG, against  $t\bar{V}$  (left) and  $t\bar{t}$  (right).

2930 to produce a discriminator with the maximum discrimination power. Table 6.10 lists  
 2931 the input variables used in the BDTG trainings for this analysis. The same set of  
 2932 input variables was used to produce the plots for MVA classifiers evaluation.

2933 Plots in Figure 6.15 shows the BDTG input variables distributions for the signal  
 2934 and background samples, in the  $3l$  channels.

2935 All the input variables have some discrimination power, however, that power is  
 2936 bigger for some of them; for instance, the third lepton  $p_T$  plot (top left in Figure 6.15)  
 2937 shows some discrimination power against WZ and VVV backgrounds for which there  
 2938 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

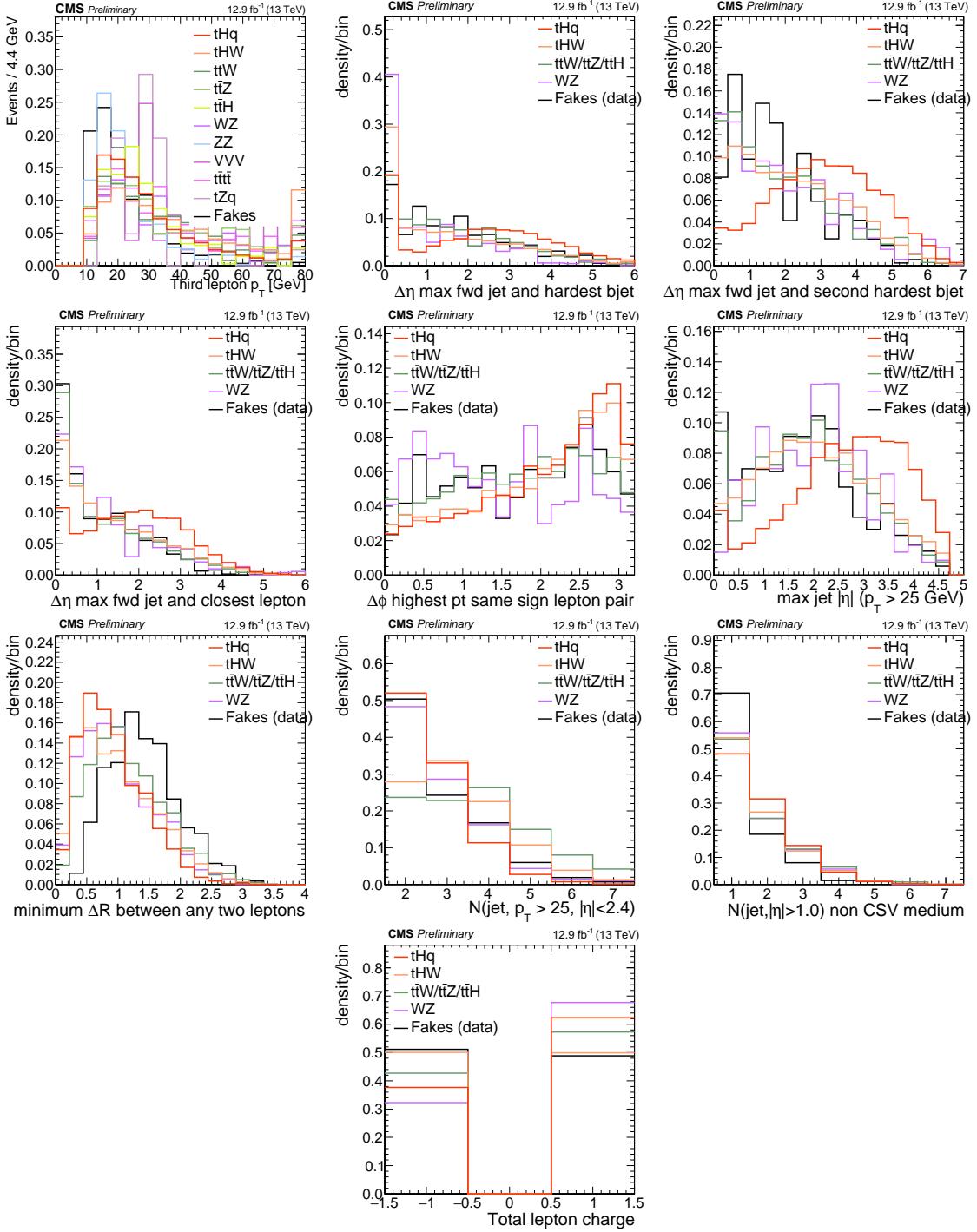
**Table 6.10:** BDTG input variables. First section lists variables related to jet multiplicities; second section lists variables related to forward jet activity, and third section lists variables related to lepton kinematics.

power does not cover all the backgrounds, it counts for the final discriminator. A similar situation can be seen in the plot for the number of jets (row three, column two);  $t\bar{t}W$ ,  $t\bar{t}Z$  and  $t\bar{t}H$  processes tend to have more jets compared to the  $tHq$  process. The discrimination power is more evident in other plots like in the plot of the maximum  $|\eta|$  of the jets in the event (row two, column three). The same or equivalent input variables are found to be performing well for both  $3l$  and  $2lss$  channels. Figure B.4 shows the corresponding input variables distribution plots for the  $2lss$  channel.

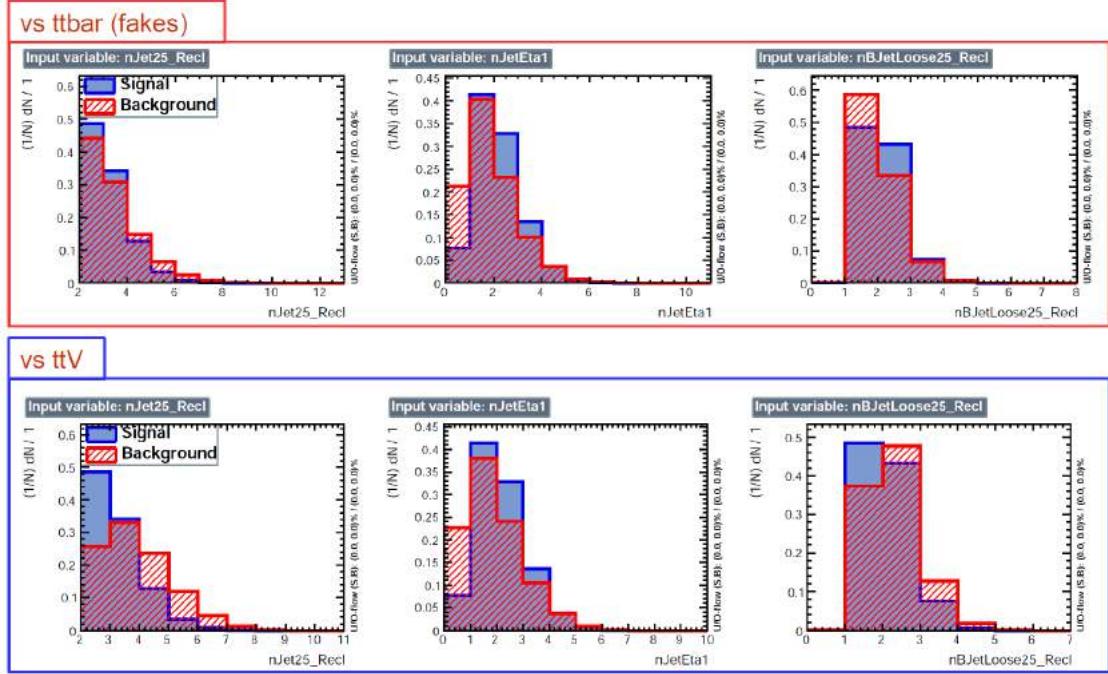
#### Discrimination power from BDTG classifier

The Discrimination power of the input variables can also be evaluated from the BDTG training, exclusively for the training samples, i.e., dominant backgrounds ( $t\bar{t}$  and  $t\bar{t}V$ ); the training samples are submitted to the selection cuts on Table 6.6.

Figure 6.16 shows the comparison between input variables for the two trainings in the  $3l$  channel; it reveals that some variables show opposite behavior for the two background sources, which results in potentially screening the discrimination power 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).

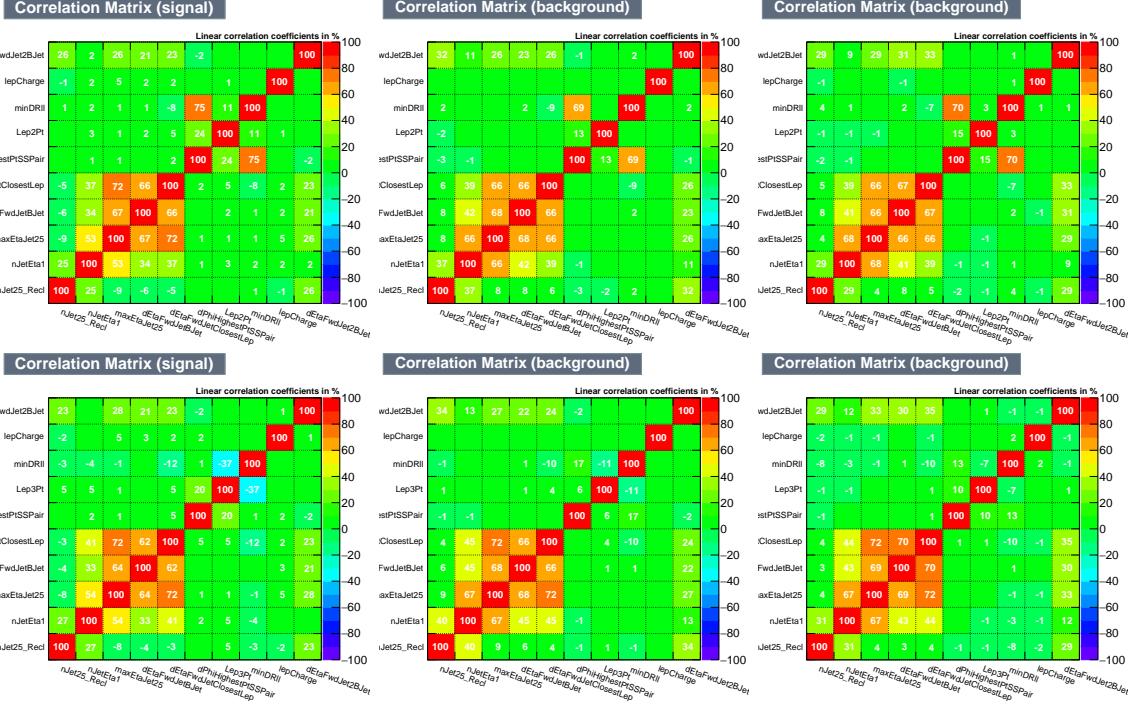
2954  $t\bar{t}V$ . For some other variables the distributions are similar in both background cases.

2955 In contrast to the distributions in Figure 6.15 only the dominant backgrounds are  
2956 included; however, the discrimination power agrees among plots.

2957 Figures in the Appendix B.5, B.6, B.7, and B.8 show the input variables  
2958 distributions for the  $2lss$  and  $3l$  channel as seen by the BDTG classifier.

### 2959 Input variables correlations

2960 From Table 6.10, it is clear that the input variables are correlated to some extent.  
2961 These correlations play an important role for some MVA methods like the Fisher  
2962 discriminant method in which the first step consist of performing a linear transfor-  
2963 mation to an phase space where the correlations between variables are removed. In  
2964 the case of BDT, correlations do not affect the performance. Figure 6.17 shows the



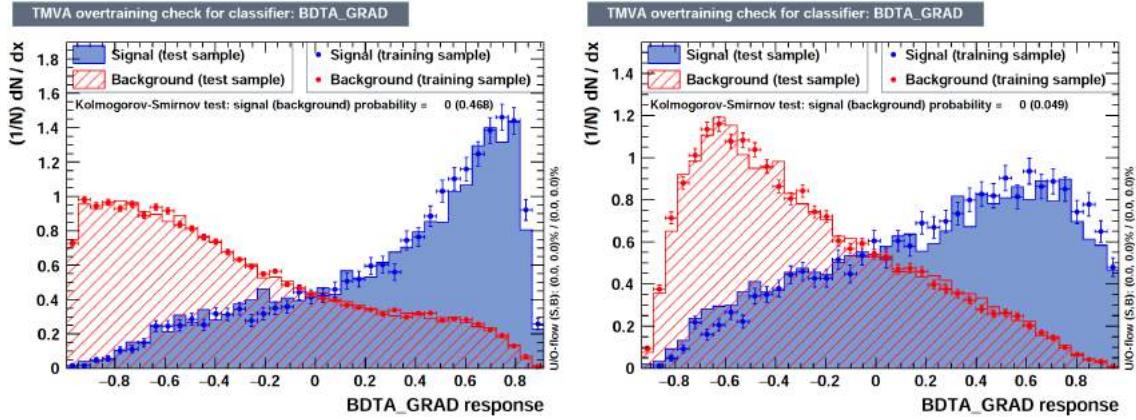
**Figure 6.17:** Signal (left),  $t\bar{t}$  background (middle), and  $t\bar{t}V$  background (right.) correlation matrices for the input variables in the BDTG classifier for the  $2lss$  (top) and  $3l$  (bottom) channels.

2965 linear correlation coefficients for signal and background for the two training cases (the  
 2966 signal values are identical by construction). As expected, strong correlations appears  
 2967 for variables related to the forward jet activity.

### 2968 6.9.3 BDTG classifiers response

2969 After the training stage, the BDTG classifier is tested to ensure its ability to discrim-  
 2970 inate between simulated signal and background events. The BDTG classifier output  
 2971 distributions for signal and backgrounds in the  $3l$  channel are shown in Figure 6.18.  
 2972 As expected, a good discrimination power is obtained using default discriminator  
 2973 parameter values; some overtraining is also visible.

2974 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.

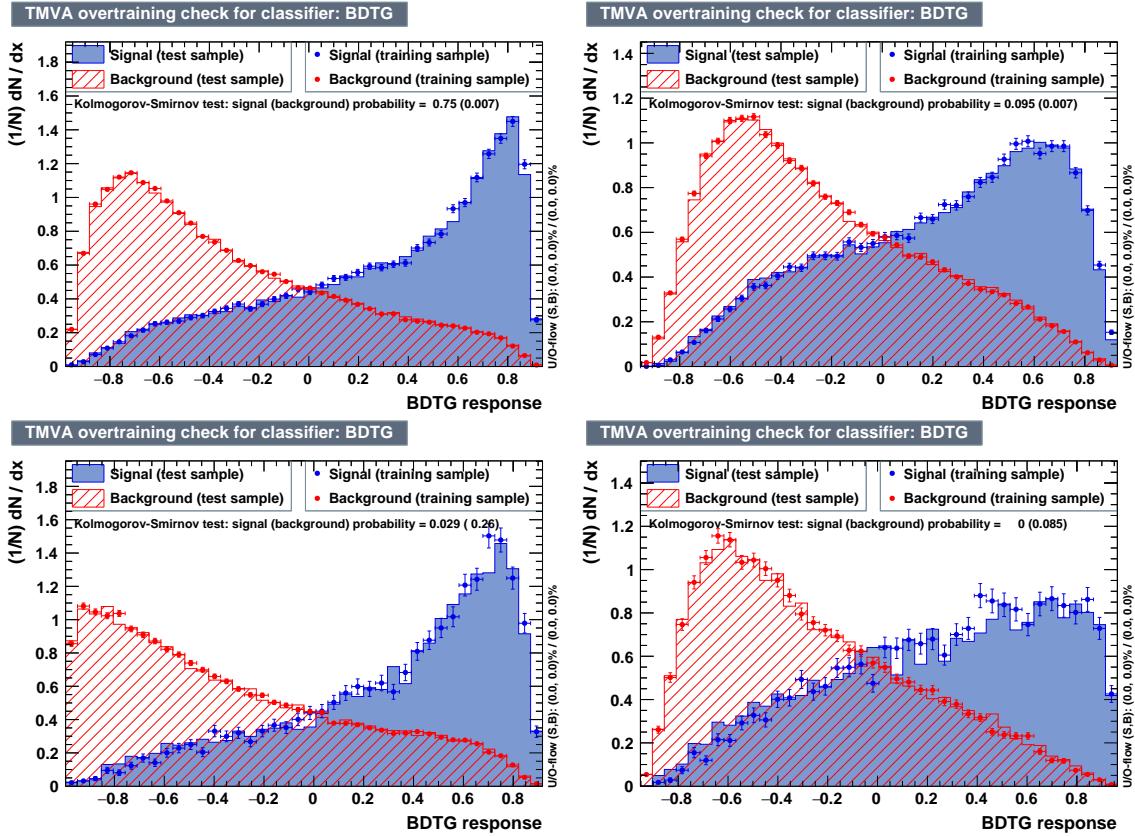
TMVA.Types.kBDT		
Option	Default	Used
NTrees	200	800
BoostType	AdaBoost	Grad
Shrinkage	1	0.1
nCuts	20	50
MaxDepth	3	

**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) .

2984 jet identification (fwdJetPUID); their distributions in the  $3l$  channel are shown in  
 2985 Figure 6.20. The forward jet identification distribution shows that for both, signal  
 2986 and background, jets are mostly originated in the primary vertex.

2987 The testing was performed by including in the BDTG input one variable at a  
 2988 time, so the discrimination power of each variable can be evaluated individually, and  
 2989 then both simultaneously. fwdJetPUID was ranked the last place in importance (11)  
 2990 in both training ( $t\bar{t}V$  and  $t\bar{t}$ ) while fwdJetPt25 was ranked 3 in the  $t\bar{t}V$  training and  
 2991 7 in the  $t\bar{t}$  training. When training using 12 variables, fwdJetPt25 was ranked 5 and  
 2992 7 in the  $t\bar{t}V$  and  $t\bar{t}$  trainings respectively, while fwdJetPUID was ranked 12 in both  
 2993 cases.

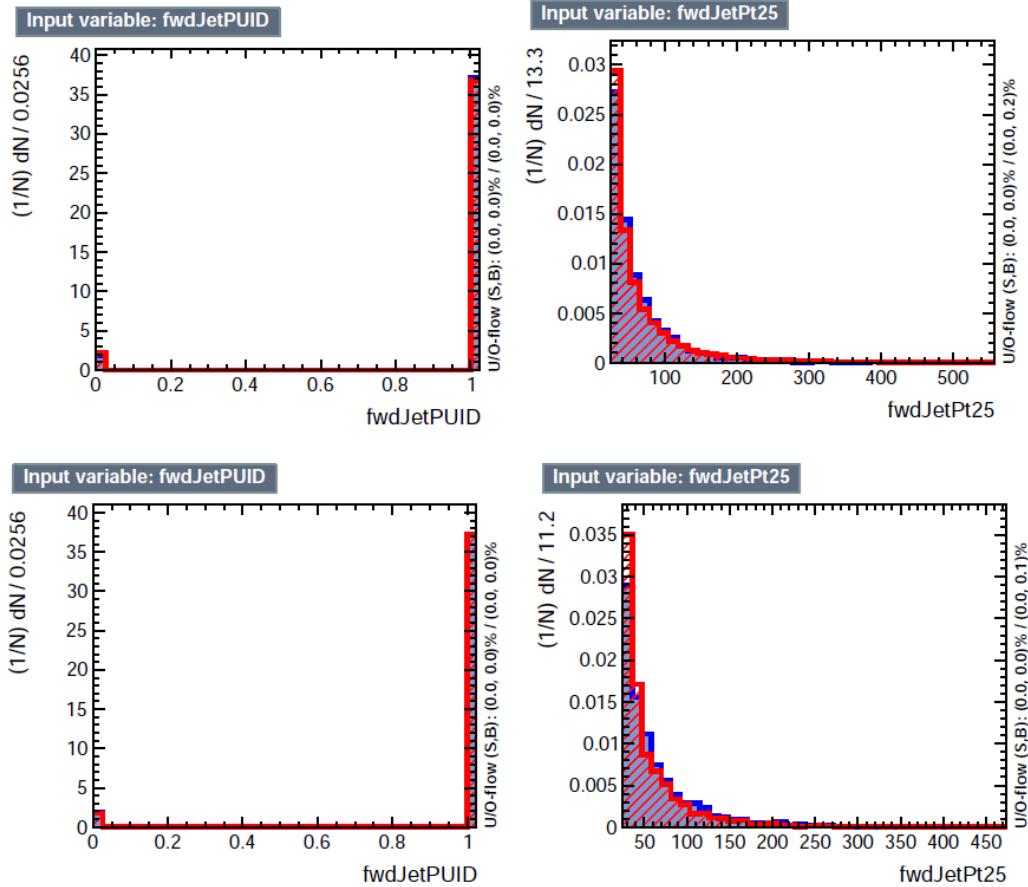
Rank	$t\bar{t}$ training	$t\bar{t}V$ training
	Variable	Variable
1	minDRll	dEtaFwdJetBJet
2	dEtaFwdJetClosestLep	Lep3Pt
3	dEtaFwdJetBJet	maxEtaJet25
4	dPhiHighestPtSSPair	dEtaFwdJet2BJet
5	Lep3Pt	dEtaFwdJetClosestLep
6	maxEtaJet25	minDRll
7	dEtaFwdJet2BJet	dPhiHighestPtSSPair
8	nJetEta1	nJet25_Recl
9	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.

2994      The improvement in the discrimination performance provided by the additional  
 2995    variables is about 1%, so it was decided not to include them in the procedure. Table  
 2996    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

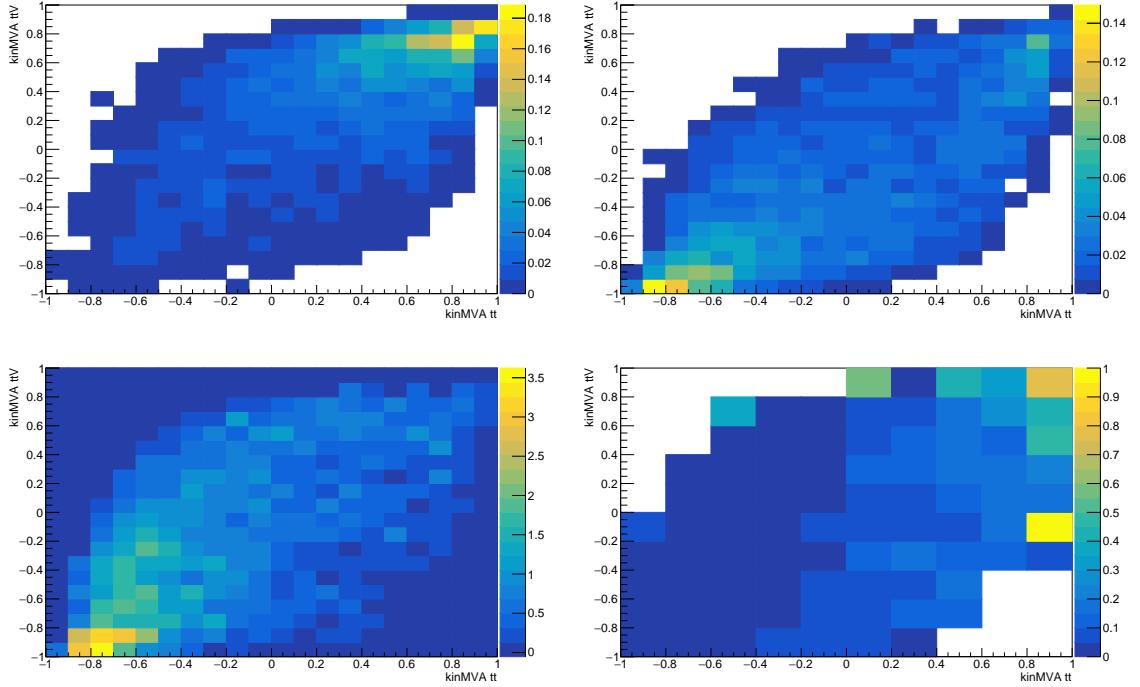
**Table 6.13:** ROC-integral for all the testing cases performed in the evaluation of the additional variables discriminating power. The improvement in the discrimination performance provided by the additional variables is about 1% .



**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.

### 2997 6.9.5 Signal extraction procedure

2998 Once the two BDTG classifiers, introduced in the previous section, are trained against  
 2999 the dominant backgrounds in each channel, they are used to classify the events in the  
 3000 samples; their outputs are then used to evaluate the signal cross section limits in a  
 3001 fit to the classifier shape. Figure 6.21 shows the expected output distributions in a  
 3002 2D plane of one training vs. the other, i.e.,  $t\bar{t}V$  vs.  $t\bar{t}$ . Top row shows the 2D planes  
 3003 for  $tHq$  and  $tHW$  signals, while the bottom left plot shows the corresponding 2D

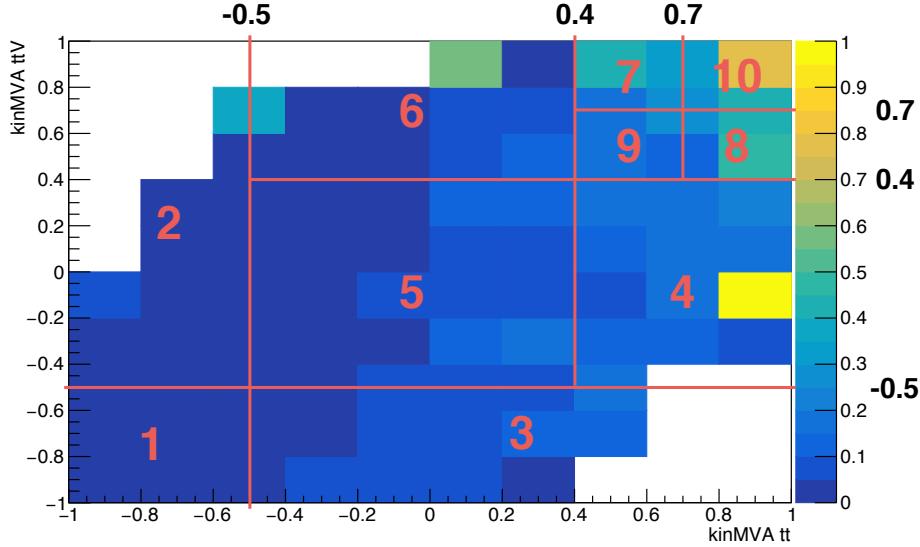


**Figure 6.21:** BDT classifier output planes (training vs  $t\bar{t}$  on x-axis and vs  $t\bar{t}V$  on y-axis) for the  $tHq$  and  $tHW$  signals (top row), and for the combined backgrounds (bottom left). Bottom right: S/B ratio (combining  $tHq$  and  $tHW$ ) in the same plane. Plots are for  $3l$  channel.

3004 plane for the combined backgrounds, which are evaluated as in the final background  
 3005 prediction, i.e., these are not the samples used in the BDTG training and this includes  
 3006 data-driven backgrounds. The signal (combining of  $tHq$  and  $tHW$ ) to background  
 3007 ratio (S/B) is showed in the bottom right plot of Figure 6.21.

3008        Each event is now classified into one of ten 2D-bins according to its position in the  
 3009 plane, as shown in Figure 6.22. The number of bins is chosen such that no bins are  
 3010 entirely empty for any process. The bin boundary positions and number of bins have  
 3011 been studied and optimized with respect to the expected limit on the signal strength  
 3012 (see Sec. 6.9.6).

3013        From this event categorization, a 1D histogram of expected distribution is pro-  
 3014 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.

3015 Asimov dataset for expected limits).

### 3016 6.9.6 Binning and selection optimization

3017 The effect of the choice of pre-selection cuts and the number of bins of the 1D his-  
 3018 togram on the cross section limit is evaluated by varying the most important cuts and  
 3019 re-calculating the limit in each case. In this analysis, the optimization was performed  
 3020 in the  $3l$  channel, by evaluating the upper limits on the  $tHq + tHW$  expected signal  
 3021 strength only (without  $t\bar{t}H$  component), always evaluated at  $\kappa_t = -1.0$ ,  $\kappa_V = 1.0$ .

3022 Table 6.14 shows several explored variations, compared with a baseline; the base-  
 3023 line is similar to the selection reported in Table 6.6 but only a loose CSV jet and a Z  
 3024 veto of  $\pm 10$  GeV are required.

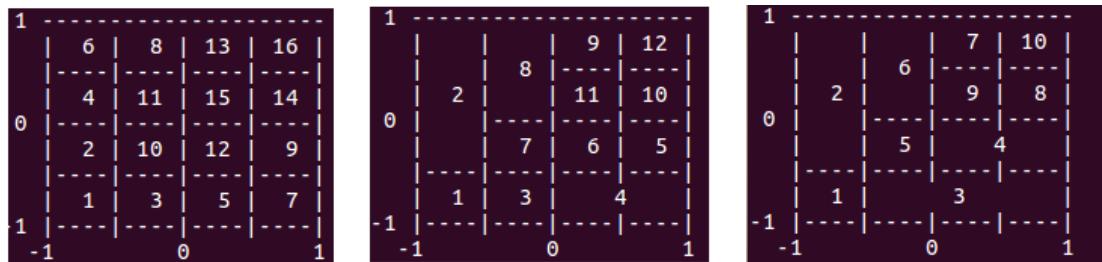
3025 The optimal limit is found when requiring a slightly tighter selection with respect  
 3026 to the baseline. The optimal selection is reported in Table 6.6.

3027 The signal strength limit also depends on the chosen binning in the 2D plane as  
 3028 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 **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.

3038 borders and the resulting signal strength limits for the same-sign dimuon channel are  
 3039 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.)

3040 The expected limit was found to be **r<1.69** for optimized bin borders in 10 bins  
 3041 and optimized pre-selection cuts.

3042 Two additional binning strategies were tested, however, the obtained limits are  
 3043 degraded; they are documented in Appendix C.

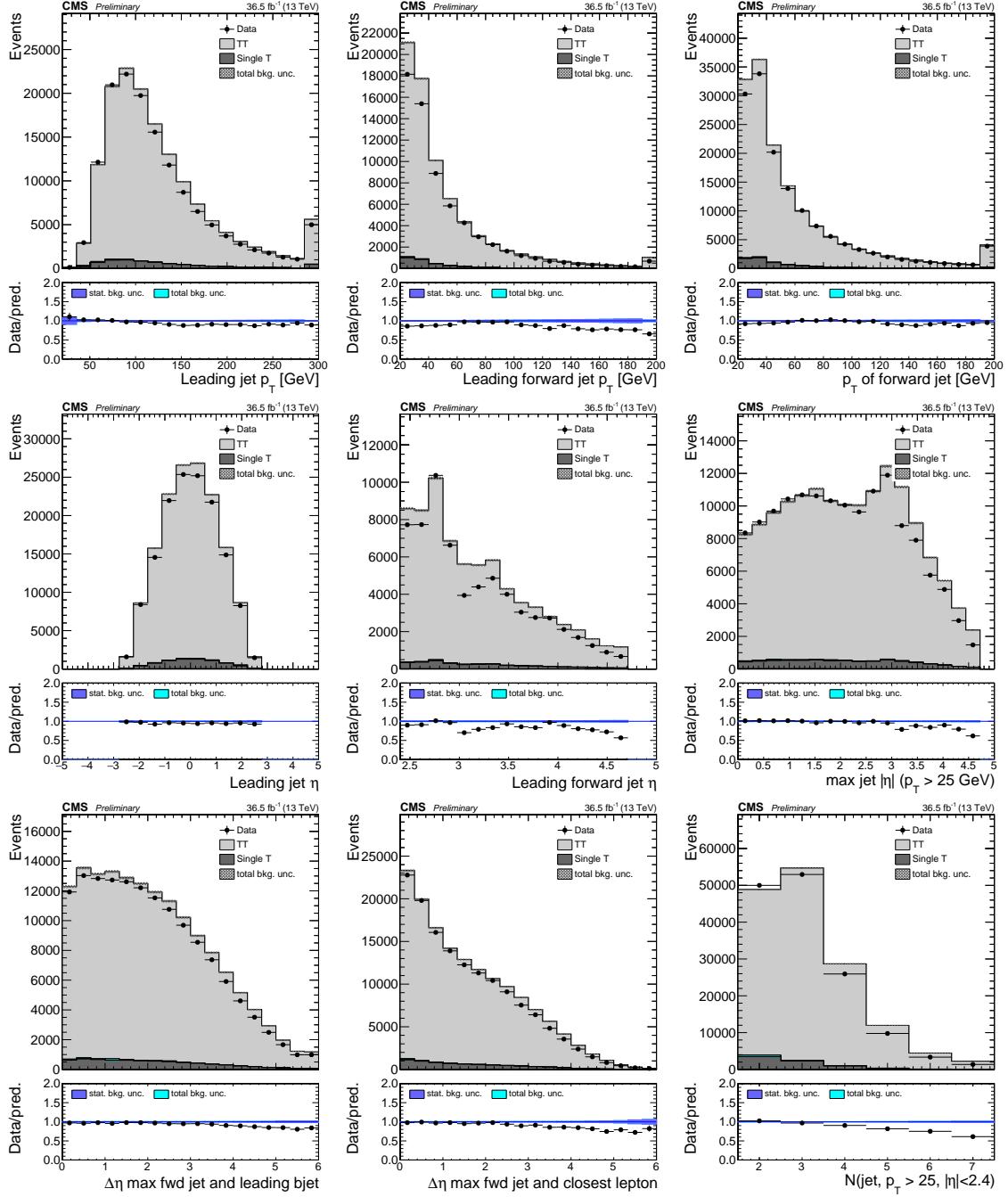
## 3044 6.10 Forward jet mismodeling

3045 As said in previous section, among the features of the  $tHq$  signature that serves as a  
 3046 powerful discriminating variable is the presence of a forward jet; unfortunately, its  $\eta$   
 3047 distribution is poorly modeled in simulation. To estimate the effect of a mismodeled  
 3048 forward jet distribution, a reweighting of the events in simulation based on the nor-  
 3049 malized data/MC ratio in a control region is performed; as a result, an alternative  
 3050 shape of the BDT output distributions that reflects a hypothetical perfect data/MC  
 3051 agreement is derived.

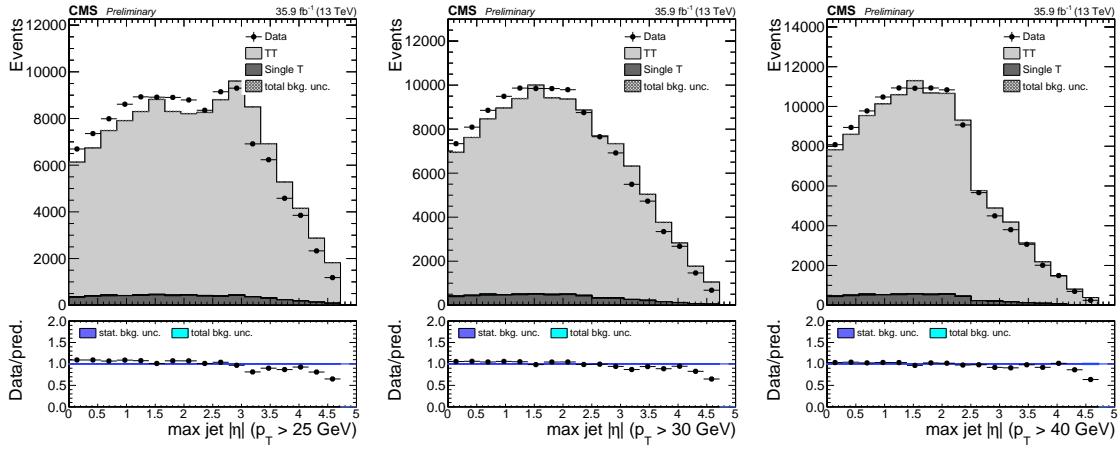
3052 Using a sample of dileptonic  $t\bar{t}$  events, the control region is defined by requiring  
 3053 two opposite-sign tight leptons in the  $e\mu$  channel, with at least two jets and at least  
 3054 one medium CSV tagged jet. (Otherwise the selection is identical to the same-sign  
 3055  $e^\pm\mu^\pm$  channel selection). Some distributions related to the forward jet for MC and  
 3056 data are shown in Figure 6.24.

3057 The disagreement of the  $\eta$  distribution of forward jets for a  $p_T$  cut of 25 GeV is  
 3058 well visible especially at higher values of  $|\eta|$ . The multiplicity for central jets is poorly  
 3059 described by the MadgraphMLM sample used here; consistent with other observations  
 3060 of the same sample. The  $t\bar{t}$  background in this analysis is modeled with a data-driven  
 3061 method and these disagreements do not directly affect the  $t\bar{t}$  contribution in the  
 3062 analysis. They do however reflect the expected agreement in these distributions for  
 3063 the irreducible backgrounds and the signal.

3064 The effect of higher  $p_T$  cuts on the forward jet has been studied for three values:  
 3065 25, 30 and 40 GeV. In order to take into account the data/MC disagreement in the  
 3066 high  $\eta$  regions, the events are weighted accordingly to the data/MC ratio of the  
 3067 unity normalized control plots shown in Figure 6.25. The data/MC agreement in the  
 3068 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  $t\bar{t}$ -enriched opposite-sign  $e\mu$  selection for the three  $p_T$  cut values studied.

3069     Table 6.17 shows the scale factors obtained for the three  $p_T$  values. The expected  
 3070     limit on cross section in the  $3l$  was used to determine the most appropriate forward  
 3071     jet  $p_T$  cut; higher  $p_T$  cut improves from 1.54 at 25 GeV to 1.51 at 30 GeV and 1.50  
 3072     at 40 GeV. The impact of the data/MC disagreement for forward jet  $\eta$  is observed  
 3073     to reduce with higher  $p_T$  cuts. Figures F.1, F.2 and F.3 show this reduction in the  
 3074     impact of the forward jet  $\eta$  nuisance in the fit.

## 3075     6.11 Signal model

3076     It is worth to remind that the main goal of this analysis is to test the compatibility  
 3077     of points in the parameter space of Higgs-to-vector boson and Higgs-to-top quark  
 3078     couplings. This is achieved by using simulated  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  signal events  
 3079     which are weighted to reflect the impact of the couplings on kinematic distributions,  
 3080     and together with different predictions of the respective production cross sections and  
 3081     branching ratios, to produce limits on the cross section for different values of  $\kappa_V$  and  
 3082      $\kappa_t$ . See Section 6.4.3 and Table A.3 for the set of  $\kappa_t$  and  $\kappa_V$  values generated. The  
 3083     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.

3084 is showed in Appendix D.

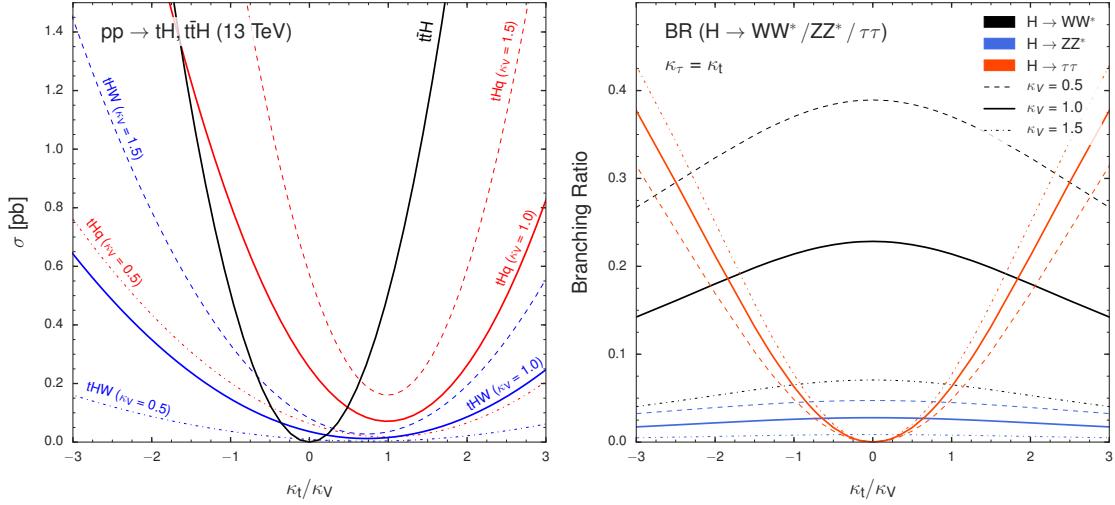
3085 In addition to the  $(\kappa_t, \kappa_V)$  dependence of the  $tHq$  and  $tHW$  production cross  
 3086 sections, due to interferences, the cross section of  $t\bar{t}H$  depends quadratically on  $\kappa_t$   
 3087 according to [158]:

$$\sigma(tHq) = (2.633\kappa_t^2 + 3.578\kappa_V^2 - 5.211\kappa_t\kappa_V) * \sigma_{SM}(tHq), \quad (6.7)$$

$$\sigma(tHW) = (2.909\kappa_t^2 + 2.310\kappa_V^2 - 4.220\kappa_t\kappa_V) * \sigma_{SM}(tHW), \quad (6.8)$$

$$\sigma(t\bar{t}H) = \kappa_t^2 * \sigma_{SM}(t\bar{t}H). \quad (6.9)$$

3088 The Higgs branching fractions to vector bosons depend on  $\kappa_V$ , and the overall



**Figure 6.26:** Scaling of the  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  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  $\kappa_V$ .

3089 Higgs decay width depend both on  $\kappa_t$  and  $\kappa_V$  when considering resolved top quark  
 3090 loops in the  $H \rightarrow \gamma\gamma$ ,  $H \rightarrow Z\gamma$ , and  $H \rightarrow gg$  decays. The relative contributions from  
 3091  $H \rightarrow WW$ ,  $H \rightarrow ZZ$ , and  $H \rightarrow \tau\tau$  also changes with changing  $\kappa_V$ .

3092 If the Higgs-to-tau coupling modifier ( $\kappa_\tau$ ) is assumed to be equal to  $\kappa_t$ , the relative  
 3093 fractions of  $WW$ ,  $ZZ$ , and  $\tau\tau$  in the event selection will only depend on the ratio of  
 3094  $\kappa_t/\kappa_V$ ; thus, any limit set at any given value of  $\kappa_t/\kappa_V$  is valid for all values of  $\kappa_t$  and  
 3095  $\kappa_V$  with that ratio, and could then be compared with theoretical predictions of cross  
 3096 sections at different values of either modifier. Figure 6.26 shows the  $tHq$ ,  $tHW$  and  
 3097  $t\bar{t}H$  cross sections(left) and the Higgs boson branching ratios  $H \rightarrow WW$ ,  $H \rightarrow ZZ$ ,  
 3098 and  $H \rightarrow \tau\tau$  (right) as a function of the  $\kappa_t/\kappa_V$  ratio.

3099 Thus, this analysis sets an upper limit on the combined cross section times branch-  
 3100 ing ratio of  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  as a function of the ratio  $\kappa_t/\kappa_V$ .

3101 Similar interpretation can be made if instead of reporting the limits as a function  
 3102 of the  $\kappa_t/\kappa_V$  ratio, they are reported as a function of the relative strength of Higgs-top  
 3103 and Higgs-vector-boson couplings, multiplied by the relative sign

$$f_t = \text{sign}\left(\frac{\kappa_t}{\kappa_V}\right) \times \frac{\kappa_t^2}{\kappa_t^2 + \kappa_V^2}. \quad (6.10)$$

3104 this parameter covers the full space between  $-1.0$  and  $1.0$ , with the SM at  $0.5$ .  
 3105 Absolute values of  $1.0$  or  $0.0$  would correspond to purely Higgs-top and purely Higgs-  
 3106 V couplings, respectively.

3107 Table 6.18 shows the points in the  $\kappa_t/\kappa_V$  and  $f_t$  parameter space that are mapped  
 3108 by the 51 individual  $\kappa_t$  and  $\kappa_V$  points.

3109 The overall Higgs decay width (modified by both  $\kappa_t$  and  $\kappa_V$ ) becomes irrelevant  
 3110 if limits are quoted as absolute cross sections rather than multiples of the expected  
 3111 cross section (which depends on it).

3112 The 1D histograms of events as categorized in regions of the 2D BDTG plane are  
 3113 then used in a maximum likelihood fit of signal and background shapes, where the  
 3114  $tHq$ ,  $tHW$ , and  $t\bar{t}H$  signals are floating with a common signal strength modifier  $r$ ,  
 3115 producing a 95% C.L. upper limit the observed cross section of  $tHq + tHW + t\bar{t}H$ .

3116 This procedure is done separately for each point  $(\kappa_t, \kappa_V)$  where the cross sections  
 3117 and branching fractions are scaled accordingly in each point. Limits at fixed values  
 3118 of  $\kappa_t/\kappa_V$  are by construction identical. Tables G.1–G.3 and G.4–G.6 in Appendix G  
 3119 show the scalings of cross section times branching fraction, as well as branching  
 3120 fractions alone for each of the Higgs decay modes and each of the signal components.

## 3121 6.12 Systematic uncertainties

3122 The uncertainties present in this analysis can be either of statistical nature given  
 3123 the size of the samples and the probabilistic nature of the processes, or of system-  
 3124 atic nature. The systematic uncertainties are associated to theoretical uncertainties  
 3125 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.

3126 tainties originating for instance from the limited resolution of the detectors. In this  
 3127 section, the contributions to the systematic uncertainties from all the sources in this  
 3128 analysis are considered.

3129        Rate uncertainties associated to the application of scaling factors for the affected  
3130    processes, and shape uncertainties which affect not only the normalization but also  
3131    the shape of certain distributions, compose the systematic uncertainties. The latter  
3132    can affect the analysis during the event selection; therefore, these systematic shape  
3133    uncertainties are applied to the simulation samples.

3134        **Experimental uncertainties.**

3135        • *Luminosity.* The measurement of the luminosity delivered by the LHC is af-  
3136    fected by experimental conditions like pileup and the number of protons per  
3137    bunch. Due to variations in the LHC running parameters an uncertainty of  
3138    2.6% is applied.

3139        • *Lepton efficiencies.* Systematic uncertainties in the signal selection efficiency  
3140    arise from correction factors applied to the simulated events in order to better  
3141    match the measured detector performance; also from theoretical uncertainties in  
3142    the modeling of the signal process. Data/MC differences in the trigger efficiency  
3143    accounted with scale factors applied to correct for them, lepton reconstruction  
3144    and identification performance, and lepton selection efficiency carry a combined  
3145    uncertainty of about 5% per lepton.

3146        • *Jets related uncertainties.* Jet energy corrections affect the uncertainty in the  
3147    signal selection efficiency it is evaluated by varying the correction factors within  
3148    their uncertainties and propagating the effects to the final results by recalculat-  
3149    ing the kinematic quantities. The effects of the jet energy scale uncertainties,  
3150     $b$ -tagging efficiency and forward jet mismodeling are evaluated using dedicated  
3151    shape templates derived from a variation of the jet energy scale within its uncer-  
3152    tainty and from varying the  $b$ -tagging forward jet data/MC scale factors within  
3153    their uncertainty.

3154       **Theory uncertainties**

3155       The uncertainties from unknown higher orders of  $tHq$  and  $tHW$  production are  
 3156       estimated from a change in the  $Q^2$  scale of double and half the initial value, evaluated  
 3157       for each point of  $\kappa_t$  and  $\kappa_V$ . The  $t\bar{t}H$  signal component has an uncertainty of about  
 3158        $+5.8/-9.2\%$  from  $Q^2$  scale variations and a further 3.6% from the knowledge of PDFs  
 3159       and  $\alpha_s$  [57]. Uncertainties related to the choice of PDF set and its scale are estimated  
 3160       to be about 3.7% for  $tHq$  and about 4.0% for  $tHW$ .

3161       The theoretical uncertainties from unknown higher orders for  $t\bar{t}W$  and  $t\bar{t}Z$  are  
 3162       12% and 10% respectively; additional uncertainties from the knowledge of PDFs and  
 3163        $\alpha_s$  of about 4% each for  $t\bar{t}W$  and  $t\bar{t}Z$  are estimated.

3164       **Backgrounds**

3165       Besides the theory uncertainties on  $t\bar{t}W$  and  $t\bar{t}Z$ , uncertainties of the smaller  
 3166       irreducible backgrounds and the charge mis-identification estimate are covered with  
 3167       flat normalization uncertainties. The  $WZ$  contribution due to the scale factor is  
 3168       derived during the background estimation using the control region.

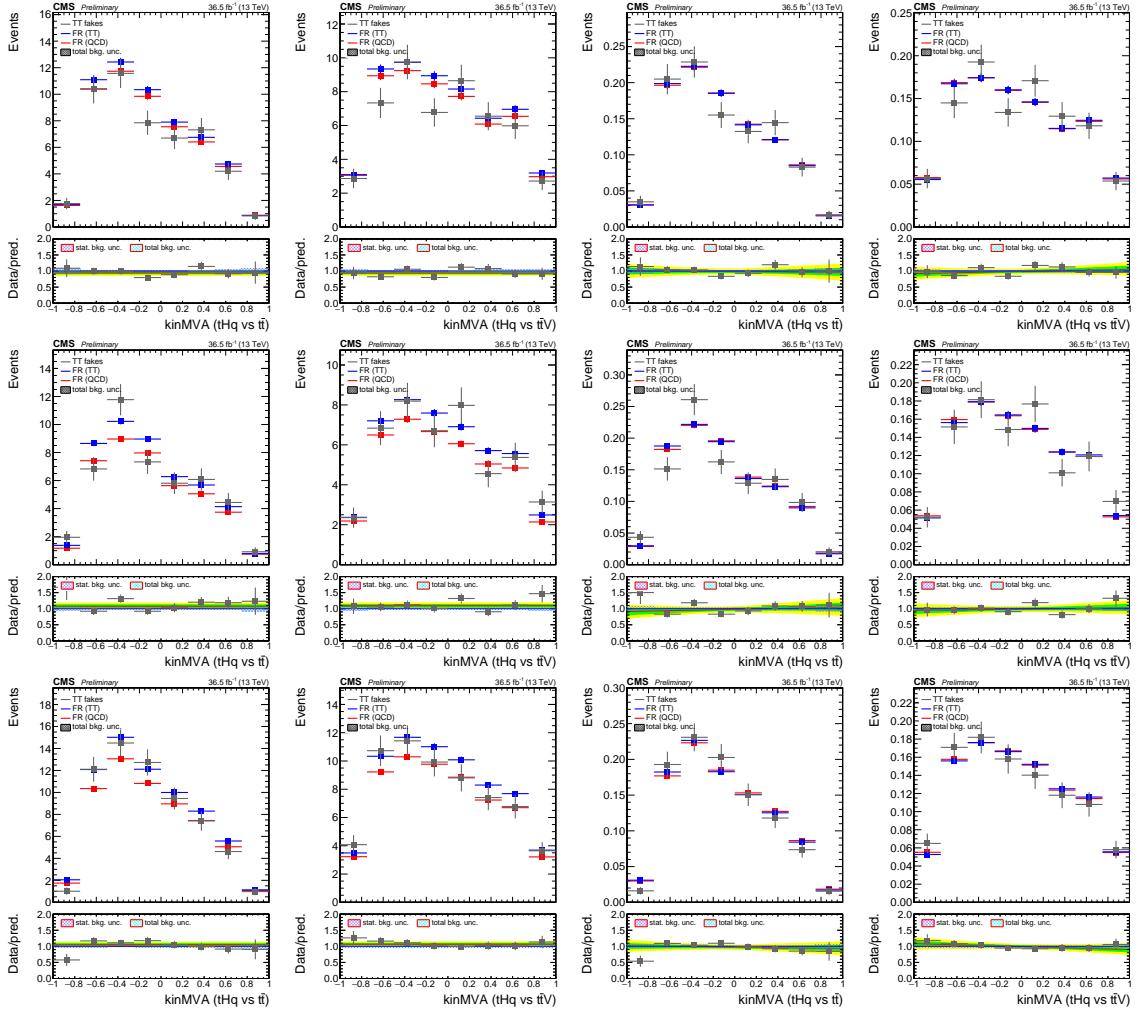
3169       The dominant uncertainty is associated to the estimate of the non-prompt lepton  
 3170       contribution using a fake rate method; the main normalization uncertainty comes from  
 3171       limited statistics in the data control region, and the subtraction of residual prompt  
 3172       lepton contribution as stated in section 6.7.2. Shape variations resembling data/MC  
 3173       differences and deviations in closure test are evaluated as shape uncertainties.

3174       **Fake rate closure uncertainties**

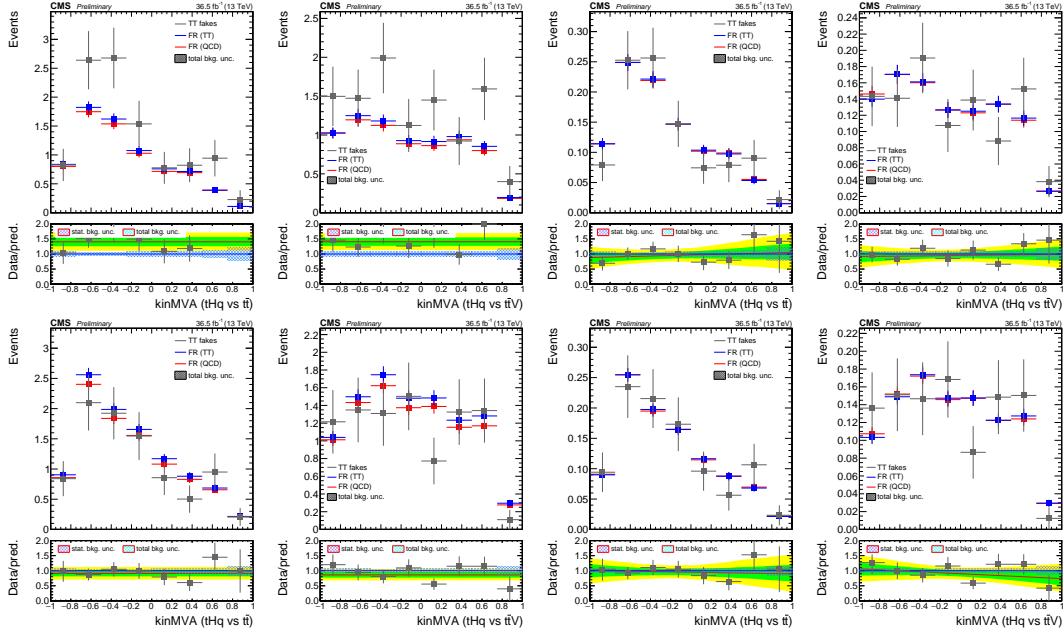
3175       In order to determine the systematic uncertainties associated to the fake rates,  
 3176       the BDTG classifier output shapes from a pure MC estimation of fake leptons (in  
 3177        $t\bar{t}$ ) and from the application of fake-rates as measured in QCD MC, applied in  $t\bar{t}$   
 3178       MC events, are compared. The difference in the resulting normalization and output  
 3179       shapes, for both trainings vs.  $t\bar{t}$  and vs.  $t\bar{t}V$ , are estimated and propagated to the

3180 fit as normalization and shape variations; Figures 6.27 and 6.28 show the results of  
3181 these closure tests.

3182 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.



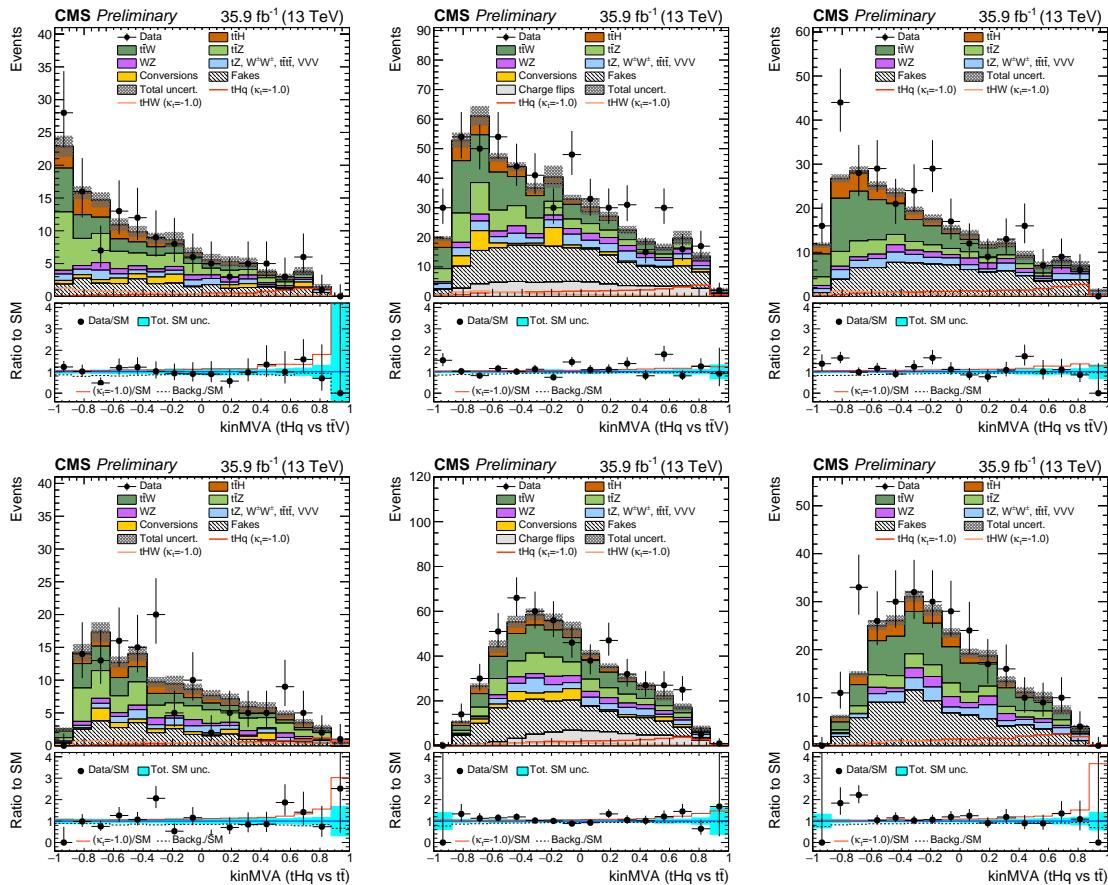
**Figure 6.28:** BDT outputs comparing  $t\bar{t}$  MC to a fake-rate prediction using fake rates measured in QCD MC. Agreement in normalization is estimated from the plots in the two left columns, shape disagreement is estimated from the (normalized) plots in the two right columns. From top to bottom 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.

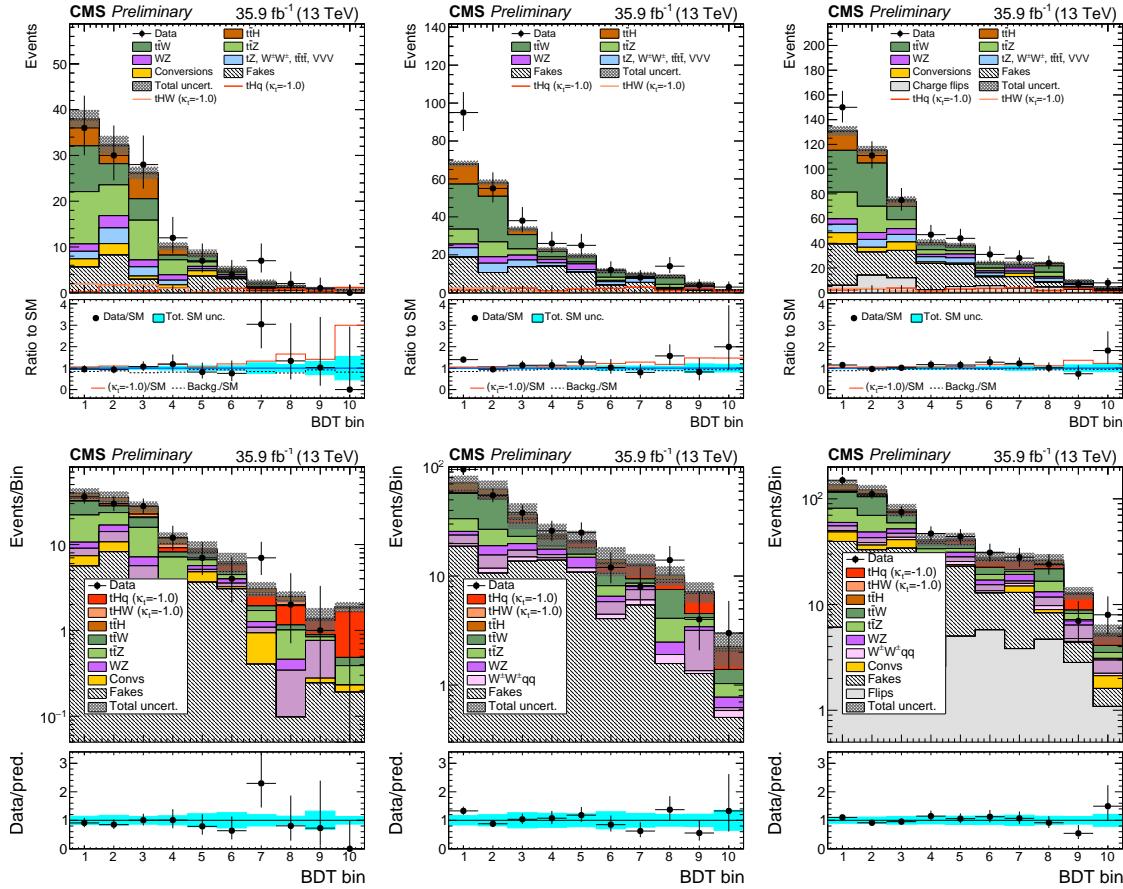
**Table 6.19:** Pre-fit size of systematic uncertainties.

## 3183 6.13 Results

3184 As a result of applying the event pre-selection on the dataset, 127 events are observed  
 3185 in the  $3l$  channel, 280 in the  $2lss \mu^\pm \mu^\pm$  channel and 525 in the  $2lss e^\pm \mu^\pm$  channel  
 3186 as shown in Table 6.8. These events are then classified into one of ten categories,  
 3187 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).

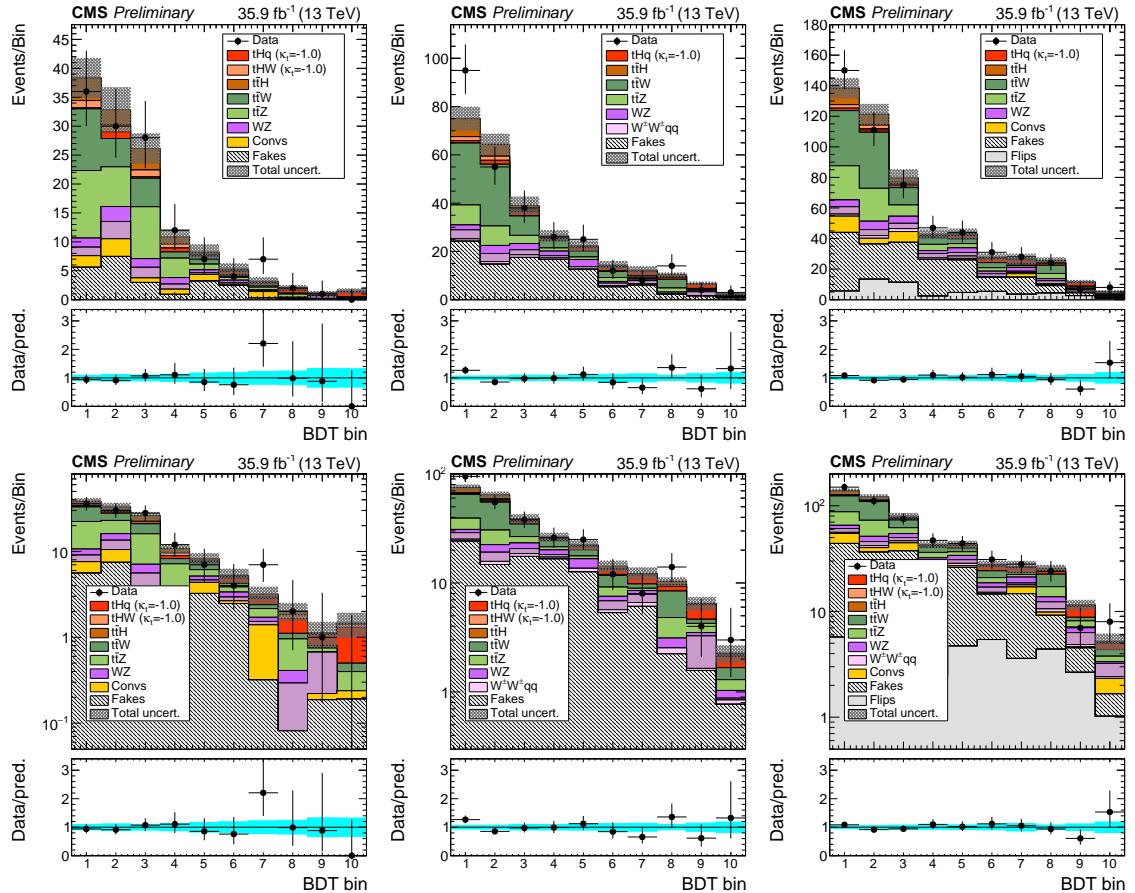
3189     The pre-fit distributions of BDTG outputs are shown in Figure 6.29, while the  
 3190     pre-fit distributions in the final binning used in the signal extraction are shown in  
 3191     Figure 6.30.

3192     The expected signal and background shapes for the distribution in the 1D his-  
 3193     togram (with ten bins) are fit to the observed data in a maximum likelihood fit, for  
 3194     all three channels simultaneously and separately for the signal shapes for each of the  
 3195     33  $\kappa_t/\kappa_V$  coupling configuration points.

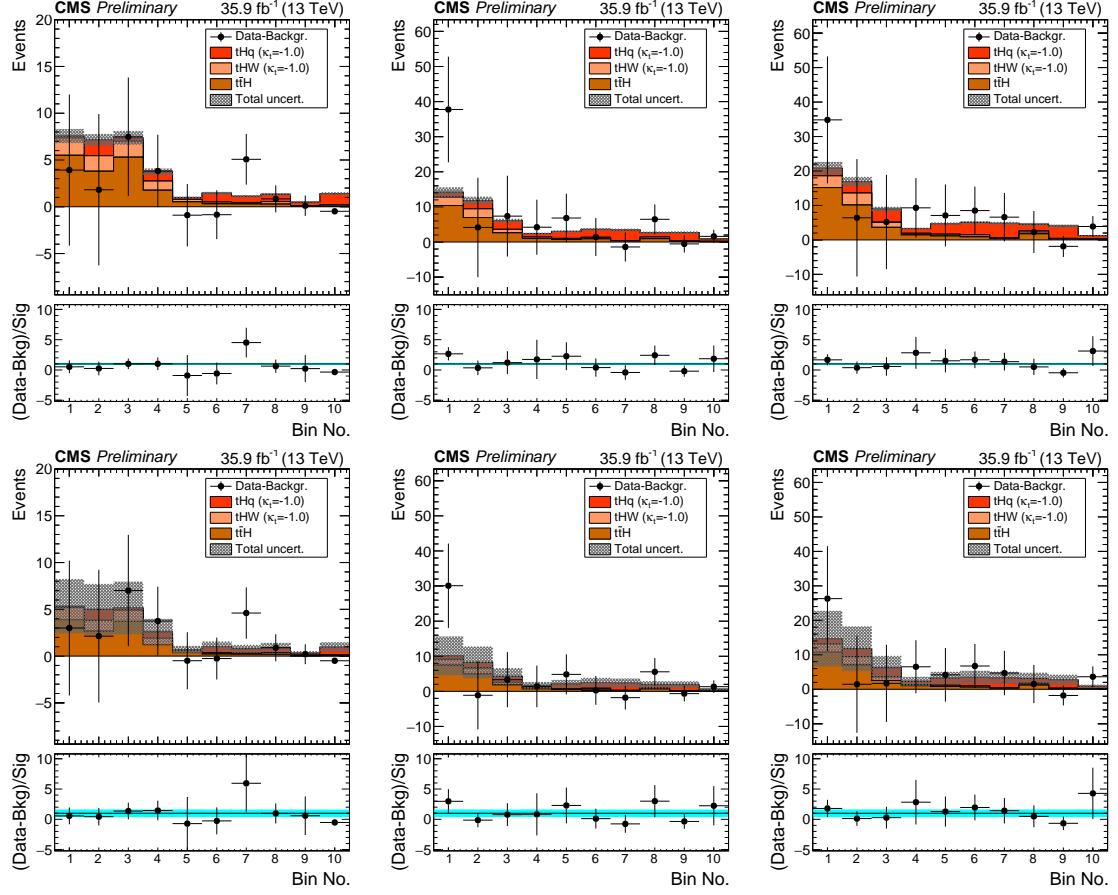
3196     The  $tH$  and  $t\bar{H}$  production cross sections and the Higgs decay branching ratios are  
 3197     modified in each point with the Higgs-top ( $\kappa_t$ ) and Higgs-vector boson ( $\kappa_V$ ) coupling

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.

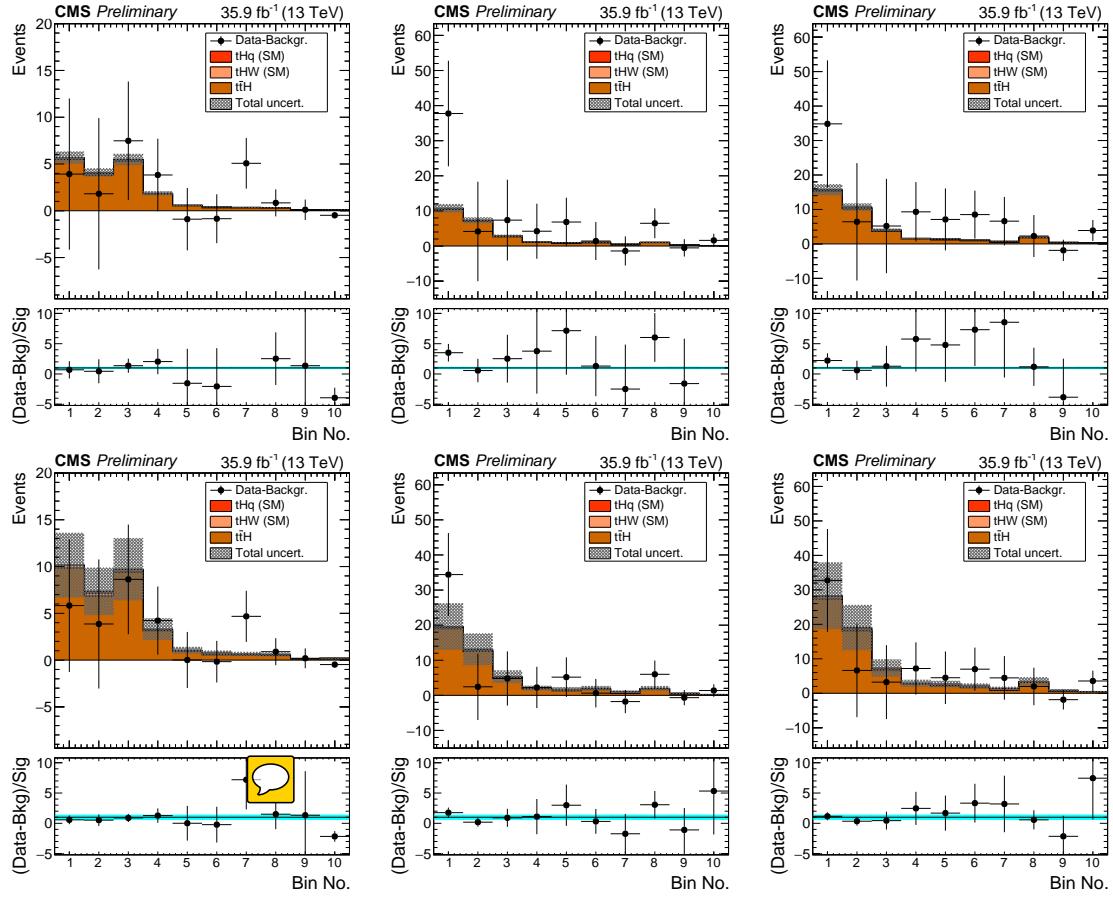


**Figure 6.31:** Post-fit distributions in the final binning used for the signal extraction, for (from left to right) the three lepton channel, the  $\mu^\pm\mu^\pm$  channel, and the  $e^\pm\mu^\pm$  channel. Linear scale (top row), and logarithmic scale (bottom row).



**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  $e^\pm\mu^\pm$  channel (right). For a fit in the inverted couplings scenario ( $\kappa_V = 1, \kappa_t = -1$ ).

3207 As expected, the signal contribution is very small compared to the back-   
 3208 ground contribution; however, it is possible to see the signal contribution by subtract-  
 3209 ing the background from the overall BDT output distributions as shown in Figure  
 3210 6.32 for the inverted coupling scenario ( $\kappa_V = 1, \kappa_t = -1$ ) and Figure 6.33 for the SM-like  
 3211 scenario ( $\kappa_V = 1, \kappa_t = 1$ ).



**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 ( $\kappa_t = \kappa_V = 1$ ).

### 3212 6.13.1 $CL_S$ and cross section limits

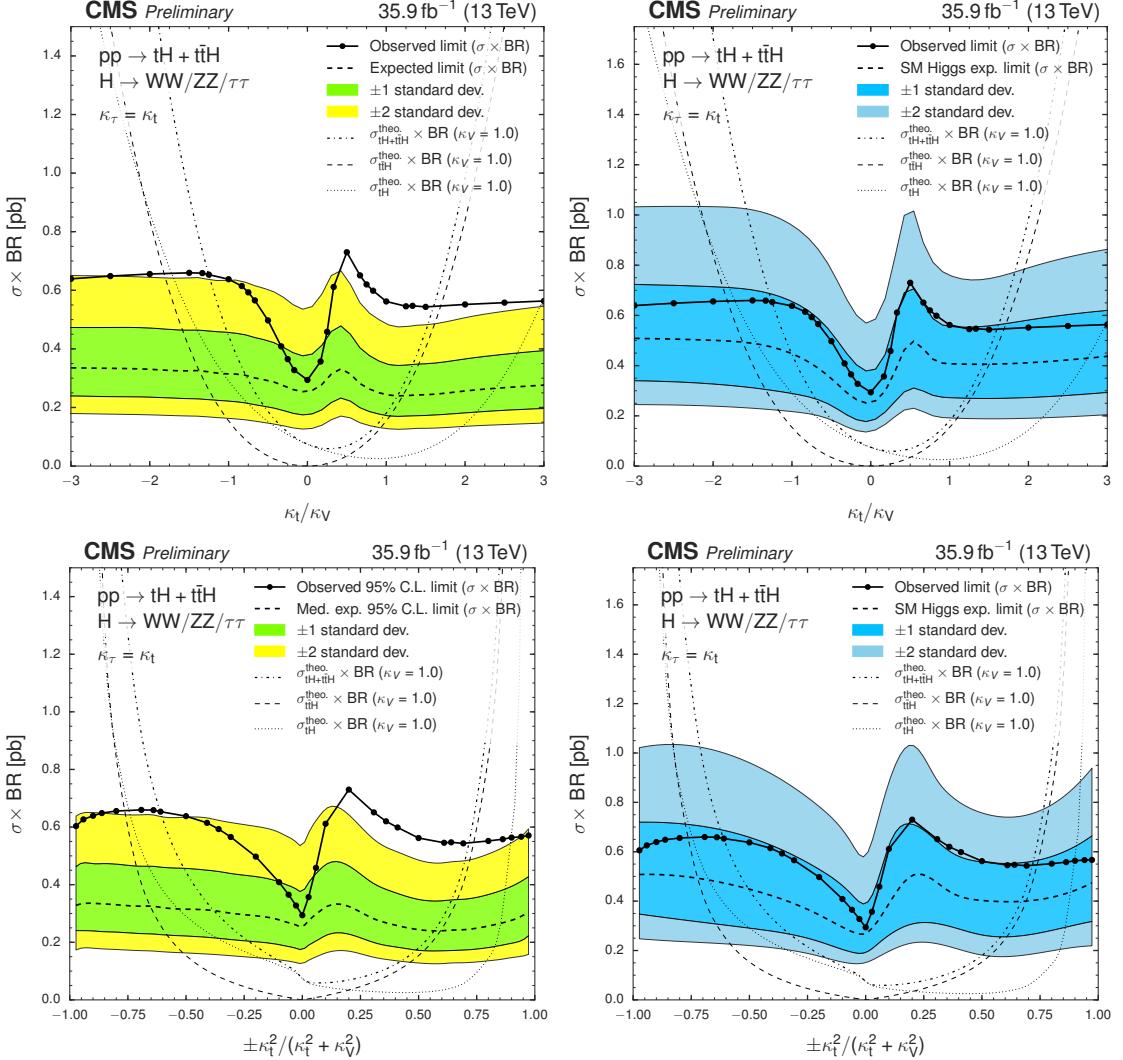
3213 Table 6.20 lists the expected background only, the expected SM-like Higgs signal, and  
 3214 the observed 95% C.L. upper limits on the  $tH + t\bar{H}$  production cross section times  
 3215  $H \rightarrow WW^* + ZZ^* + \tau\tau$  branching ratio (in pb); the corresponding plots are shown  
 3216 in Figure 6.34 for  $\kappa_V = 1$ . The expected background-only limit is calculated on an  
 3217 Asimov dataset, while the expected SM-like limit is calculated on an Asimov dataset  
 3218 that includes the SM-like  $tH$  and  $t\bar{H}$  signals.

3219 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 $^{+0.007}_{-0.008}$

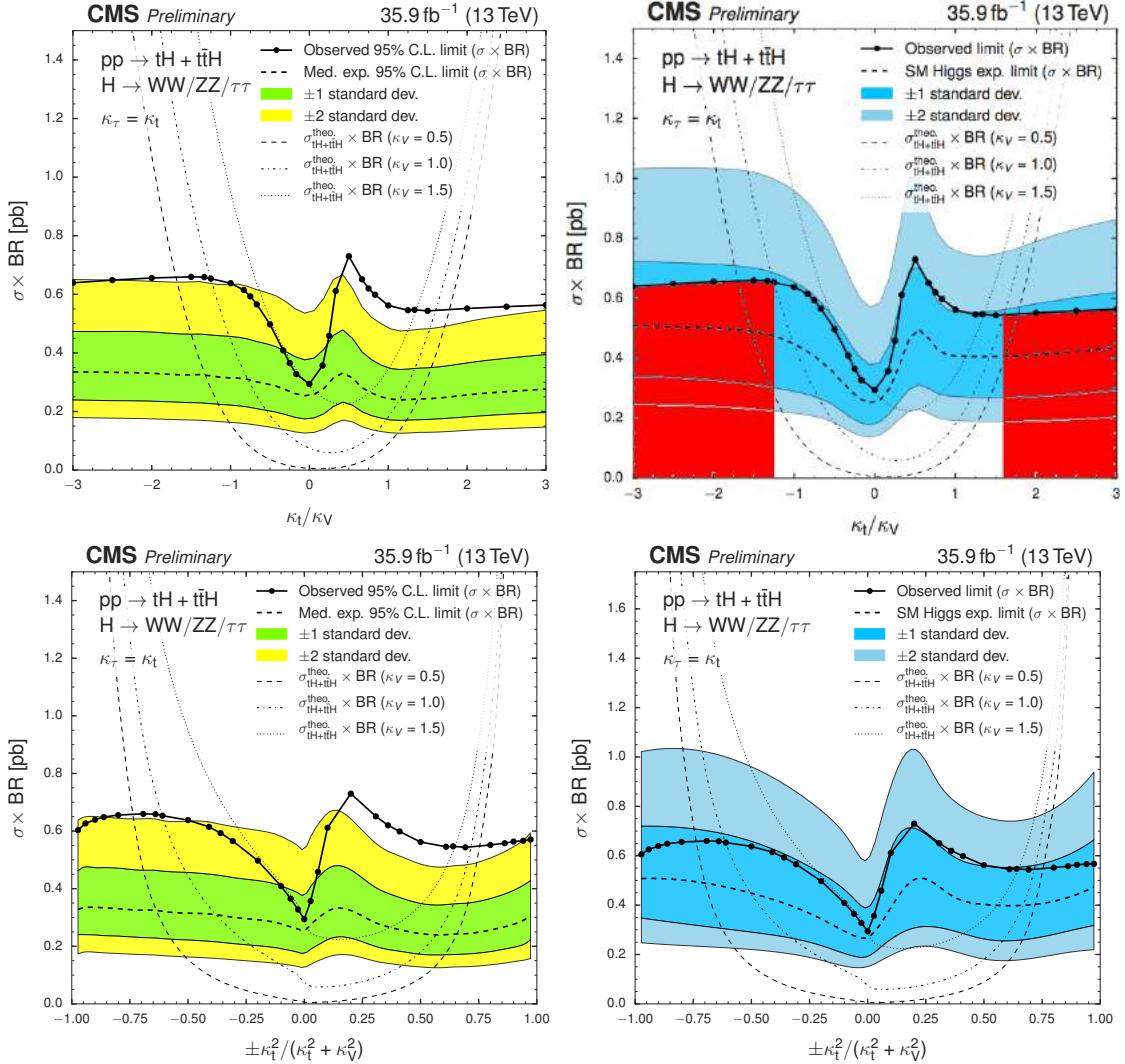
**Table 6.20:** Expected (for background only, and for a SM-like Higgs signal) and observed 95% C.L. upper limits (in pb), and best fit signal strength  $r$  and corresponding best fit cross section for the combined  $tH + t\bar{t}H$  cross section times modified branching ratio for the combination of 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.

3224 deviation of the observed limit from the expected one is much smaller than  $1\sigma$ ; this is  
 3225 consistent with the results presented in Reference [149]. It is also evident that, given  
 3226 the dependence of the  $t\bar{t}H$  cross section on  $\kappa_t^2$ , the source of the asymmetry in both,  
 3227 background-only and SM-like, limits is induced by the  $tH$  component of the signal.  
 3228 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.

3229     $t\bar{t}H$  cross section times BR for  $\kappa_V = 1.0$  constrains the allowed range of coupling  
 3230    configurations  $\kappa_t/\kappa_V$  to between about -1.25 and +1.60. as shown in the top right  
 3231    plot in Figure 6.35.

3232    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

6.21, whereas, the summary of the 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 thereof, for the ITC and SM-like scenarios are presented in  
 Table 6.26.

### 6.13.2 Best fit

The best-fit results for the signal strength in all the 33  $\kappa_t/\kappa_V$  configurations are also listed in Table 6.20; the inverted top coupling (ITC) and the SM-like scenarios are highlighted there and summarized in Table 6.23. The individual contributions from all the channels to the best-fit signal strength for the SM-like Higgs signal are listed 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	$2.73\sigma(1.50\sigma)$

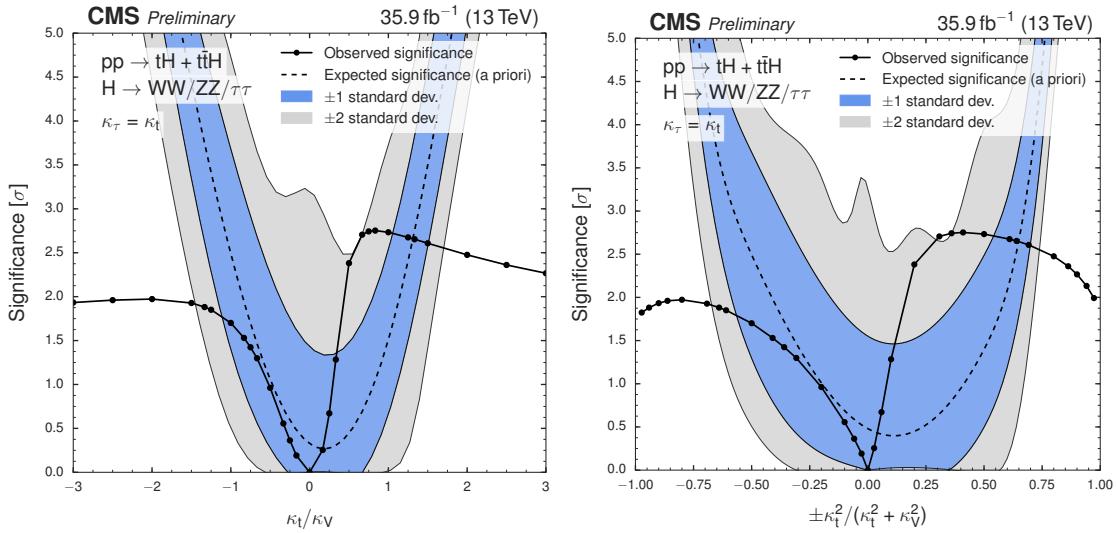
**Table 6.23:** Best fit for signal strength  $r$  and corresponding best fit cross section for the combined  $tH + t\bar{t}H$  cross section times modified branching ratio for the combination of all three channels, for the ITC and the SM-like scenarios.

$\ell\ell\ell$	$r = 1.44_{-0.84}^{+0.91}$
$e^\pm \mu^\pm$	$r = 1.42_{-1.03}^{+1.06}$
$\mu^\pm \mu^\pm$	$r = 2.75_{-1.11}^{+1.22}$
Combined	$r = 1.82_{-0.69}^{+0.76}$
Expected	$r = 1.00_{-0.65}^{+0.70}$

**Table 6.24:** Best-fit signal strengths for a SM-like Higgs signal for the individual channels.

In the SM scenario, a signal strength of 1.82 is obtained which corresponds to a cross section of 0.33 pb. The observed significance of the signal, in a background-only hypothesis, is  $2.7\sigma$ , with an a-priori expected significance of  $1.5\sigma$ . For the ITC scenario, the best fit signal strength is 0.68, corresponding to a significance

3252 of  $1.7\sigma$  (5 $\sigma$  expected); a scan of the observed and expected significances over the  
 3253  $\kappa_t/\kappa_V$  configurations is shown in Fig. 6.36. Note that the fit favors a signal strength  
 3254 compatible with zero for a scenario with  $\kappa_t = 0$  (where the  $t\bar{t}H$  component vanishes).

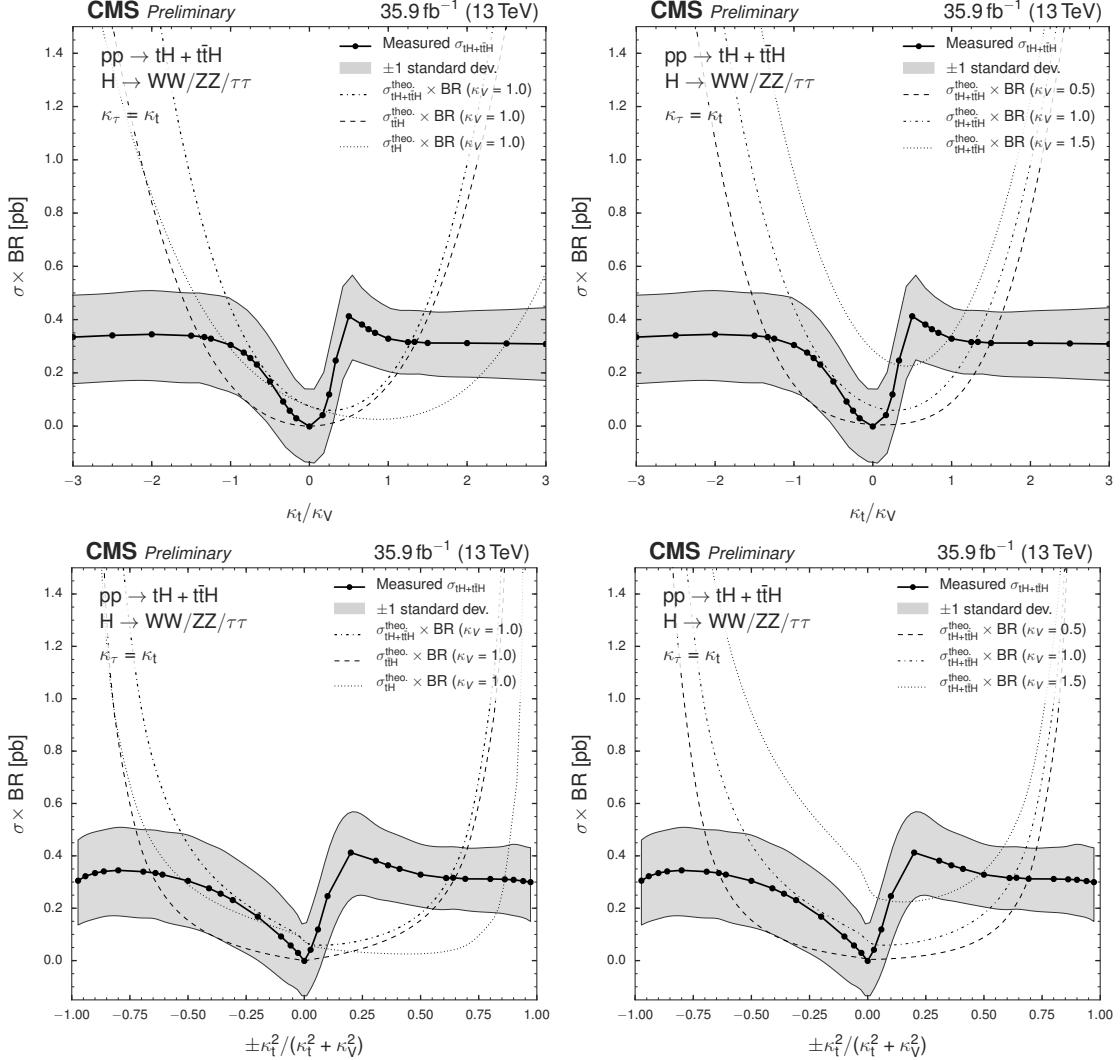


**Figure 6.36:** Observed and a priori expected significance of the fit result (in a background-only hypothesis) as a function of  $\kappa_t/\kappa_V$  (top) and  $f_t$  (bottom) for the combination of three lepton channel,  $\mu^\pm\mu^\pm$ , and  $e^\pm\mu^\pm$  channel.

3255 A scan over the best fit values of the combined cross section times modified BR is  
 3256 shown in Figure 6.37. The fact that the best fit signal strength at  $\kappa_t = 0$ , where the  
 3257  $t\bar{t}H$  component of the signal is zero, is compatible with zero implies that the best fit  
 3258 for the cross section is also compatible with zero, which again reveals that the excess  
 3259 in the cross section limit with respect to the expectation is not  $tH$ -like but  $t\bar{t}H$ -like.

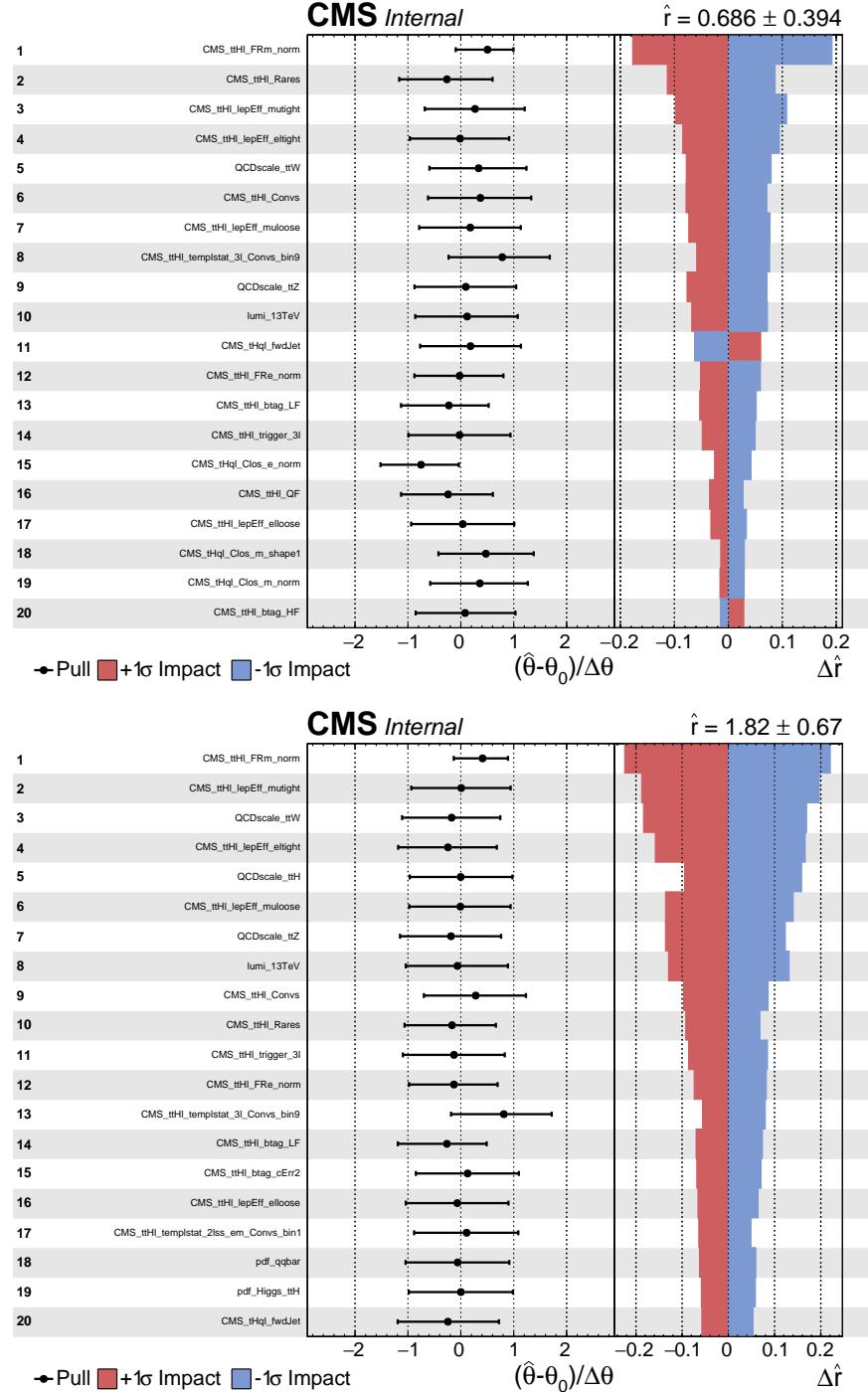
### 3260 6.13.3 Effect of the nuisance parameters

3261 The post-fit behavior of the most important nuisance parameters is presented in the  
 3262 pulls and impacts plots in Figures B.9, B.9 and B.9; additional pulls and impacts  
 3263 can be found in Appendix B.4

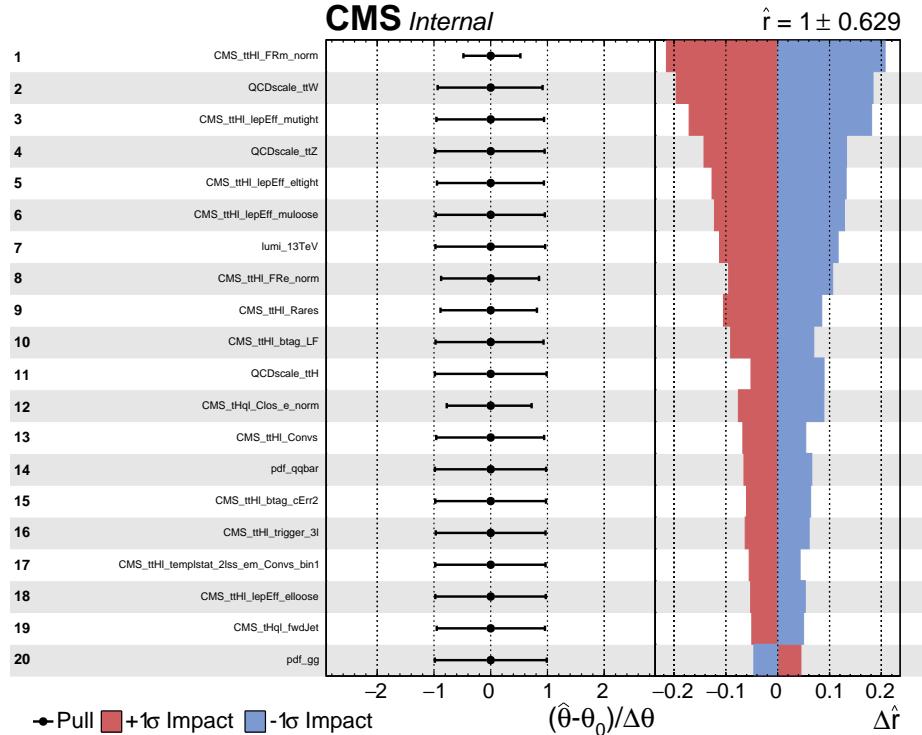


**Figure 6.37:** Best fit values of the combined  $tH + t\bar{H}$  cross section times modified BR as a function of  $\kappa_t/\kappa_V$  (top) and  $\text{sign}(\kappa_t/\kappa_V) \times \frac{\kappa_t^2}{(\kappa_t^2 + \kappa_V^2)}$  (bottom) for the combination of three lepton channel,  $\mu^\pm\mu^\pm$ , and  $e^\pm\mu^\pm$  channel.

3264     Most of the nuisance parameters stay close to their initial values. The biggest  
 3265     impact on the signal strength limits is associated to the fake rates for muons, followed  
 3266     by the lepton efficiencies and nuisances associated to the QCD scales. The lower  
 3267     impact in the ITC scenario is associated to the b-tag and  $tHq$  closure normalization  
 3268     and shape nuisances, while in the SM scenario, nuisances associated to the forward  
 3269     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.

## 3274 6.14 CP-mixing in $tHq$

3275 The sensitivity of the  $tH$  production process to the CP-mixing in the Higgs boson  
 3276 sector was explored in Section 1.6; the theoretical model postulates the existence of a  
 3277 generic spin-0 particle  $X_0$  with CP-symmetry violating interaction with the top quark  
 3278 but SM-like interaction with the W boson.

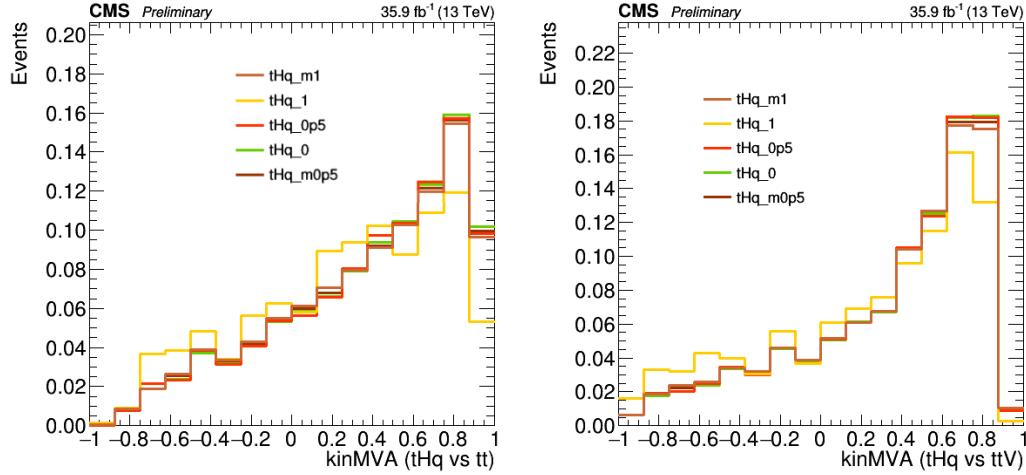
3279 The LHE reweighting procedure used in the ITC analysis is used in this CP-

$\cos(\alpha_{CP})$	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.

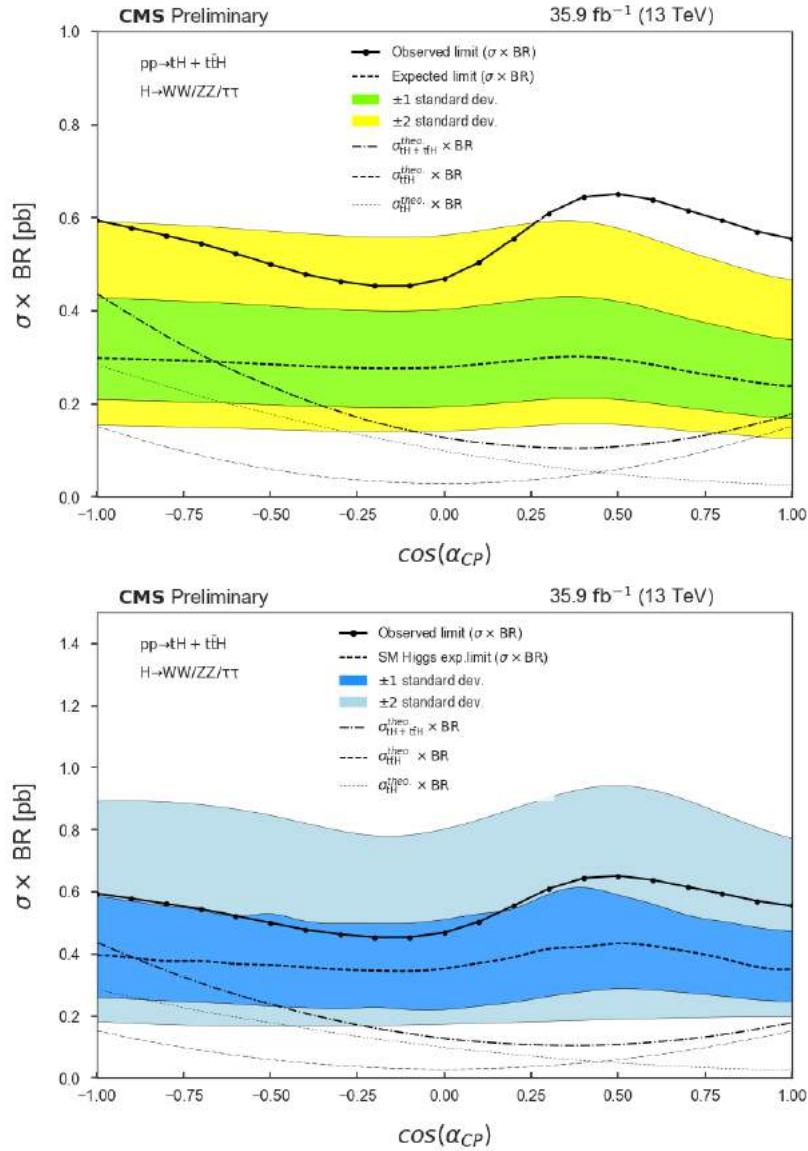


**Figure 6.40:** BDT shape variations for five CP-mixing angles. The trainings use the same set of input variables and samples as for the  $\kappa_t$ - $\kappa_V$  study. Since there are big variations between BDT output, only training was performed.

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  $t\bar{t}H$  [?]  $tH$  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.

3304 Table 6.26 summarizes the upper limits for the ITC ( $\cos(\alpha_{CP}) = -1$ ), SM ( $\cos(\alpha_{CP}) =$   
 3305 1), and fully pseudo-scalar ( $\cos(\alpha_{CP}) = 0$ ) CP-mixing configurations.

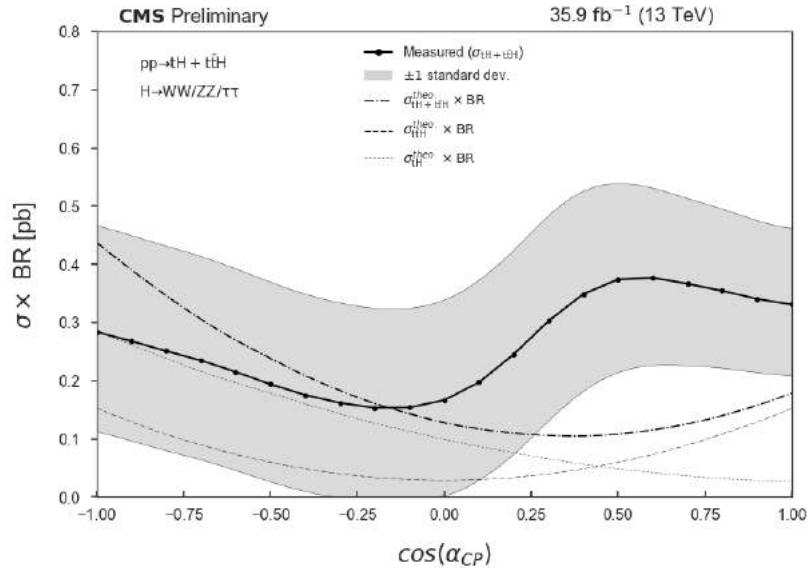
3306 The CP-mixing limits are consistent with the limits obtained in the  $\kappa_t$ - $\kappa_V$  anal-  
 3307 ysis as expected; however, in the CP-mixing case it is not possible to exclude any

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, an  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  $tH + t\bar{H}$   $\sigma \times \text{BR}$  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.

<sub>3316</sub> **Chapter 7**

<sub>3317</sub> **Phase 1 FPix upgrade modules**

<sub>3318</sub> In chapter 2, a description of the CMS pixel detector used during the collection  
<sub>3319</sub> of the data sets used in this analysis, was presented. During the extended year-end  
<sub>3320</sub> technical stop (EYETS) 2017, the complete CMS pixel detector was replaced in order  
<sub>3321</sub> to support the full performance of the CMS experiment under the higher radiation  
<sub>3322</sub> conditions produced by the increasing instantaneous luminosity delivered by the LHC  
<sub>3323</sub> accelerator. It also was designed to address and mitigate the identified weaknesses in  
<sub>3324</sub> the previous system.

<sub>3325</sub> In this chapter, a description of the upgraded detector will be presented. Emphasis  
<sub>3326</sub> will be put on the contributions made by the University of Nebraska - Lincoln (UNL)  
<sub>3327</sub> HEP group, which consisted of the assembly of about 600 of the modules that make  
<sub>3328</sub> up the phase 1 upgraded forward pixel detector (FPix); in particular, the gluing and  
<sub>3329</sub> encapsulation stages will be described in detail since they are my contributions. A  
<sub>3330</sub> complete description of the upgrade design and plans is presented in Reference [?]  
<sub>3331</sub> which is the main source of the information contained in this section unless additional  
<sub>3332</sub> references are provided.

## 3333 7.1 CMS pixel detector upgrade

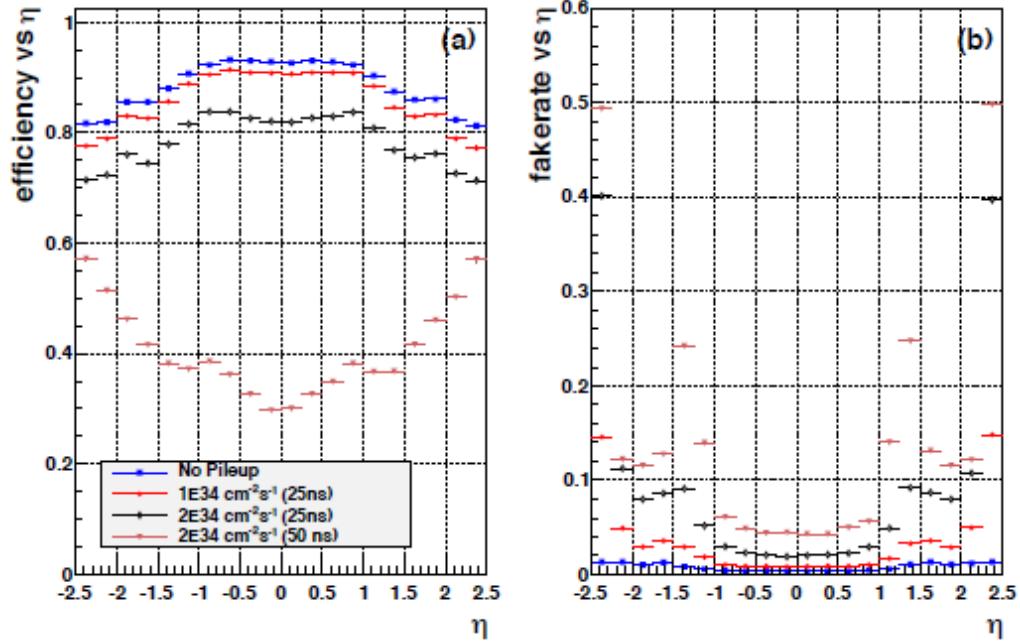
3334 The previous pixel detector was designed to record efficiently and with high precision  
 3335 the first three space-points near the interaction region, in the range of  $|\eta| < 2.5$ , at  
 3336 a instantaneous luminosity of  $1 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$  and a bunch crossing each 25 ns.  
 3337 An average pileup of about 25 simultaneous overlapping events is expected. The  
 3338 increasing luminosity would affects the performance of the detector reducing track  
 3339 reconstruction efficiency, and increasing the data loses caused by the degradation of  
 3340 the readout system; furthermore, if the LHC runs with 50 ns bunch spacing at twice  
 3341 the luminosity, then the data losses would increase almost exponentially, to losses of  
 3342 50% for the innermost layer. An illustration of the foreseen reduced performance in  
 3343 tracking efficiency and data loss is shown in Figure 7.1 in the case of simulated  $t\bar{t}$   
 3344 events at instantaneous luminosities up to  $2 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$  with 25 ns and 50 ns  
 3345 bunch spacing. The increasing fake rate is also showed. In conclusion, the prevoius  
 3346 pixel detector was not able to perform efficiently under the new luminosity, pileup,  
 3347 radiation, and running conditions.

3348 The present system is designed to offer high performance under these new oper-  
 3349 ational conditions; it is composed of four-layers/three-disks, low mass silicon pixel  
 3350 detectors providing a high performance tracking in the high luminosity environment.  
 3351 The design was leaded by the following requirements<sup>1</sup>

- 3352     • In running with 50 or more pile-up, maintain the high efficiencies and low fake  
   3353        rates.
- 3354     • New pixel readout chip (ROC) to minimize data loss due to latencies and limited  
   3355        buffering in high luminosity running.

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<sup>1</sup> Taken literally from the technical design report.



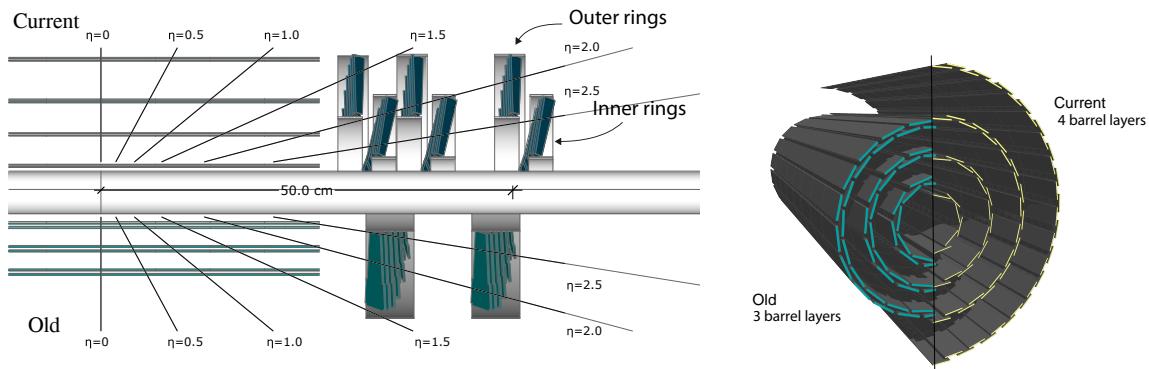
**Figure 7.1:** Expected performance of the previous pixel detector in simulated  $t\bar{t}$  events: a) efficiency; b) fake rate. Conventions are the same for both plots, considering zero pileup (blue squares), average pileup of 25 (red dots), average pileup of 50 (black diamonds), and average pileup of 100 (magenta triangles).

- 3356     • Minimize degradation due to radiation damage.
- 3357     • Optimized detector layout for 4-pixel-hit coverage over the  $\eta$  range with minimal  
3358       innermost layer radius improving pattern recognition and track reconstruction.
- 3359     • To reduce material, adopt two-phase  $CO_2$  cooling and light-weight mechani-  
3360       cal support, moving the electronic boards and connections out of the tracking  
3361       volume.
- 3362     • To reuse the current patch panel and off-detector services, cooling pipes, cables  
3363       and fibers, adopt DC-DC power converters and higher bandwidth electronics.
- 3364     • Reduce number of module types and interfaces simplifying production and main-  
3365       tenance.

3366     • New smaller diameter beam pipe to accommodate the placement of the inner  
 3367       pixel layer closer to the interaction region.

3368       The upgraded detector is expected to provide higher efficiencies, lower fake rates,  
 3369       lower dead-time/data-loss, and an extended lifetime of the detector, which translate  
 3370       in better muon ID, b-tagging, photon/electron ID, and tau reconstruction, in both  
 3371       HLT and offline levels. No details about the performance of the current pixel detector  
 3372       are given here since that matter falls beyond the purpose of this document; however,  
 3373       it is documented in Reference [159].

3374       Figure 7.2 shows the layout of the upgraded pixel detector. The old 3-layer barrel  
 3375       (BPIX), 2-disk endcap (FPix) system is replaced with a 4-layer barrel, 3-disk endcap  
 3376       system. The additional barrel layer and forward disk provide redundancy for the  
 3377       track pattern recognition and reconstruction.



**Figure 7.2:** Layout and comparison of the layers and disks in the current and old pixel detectors.

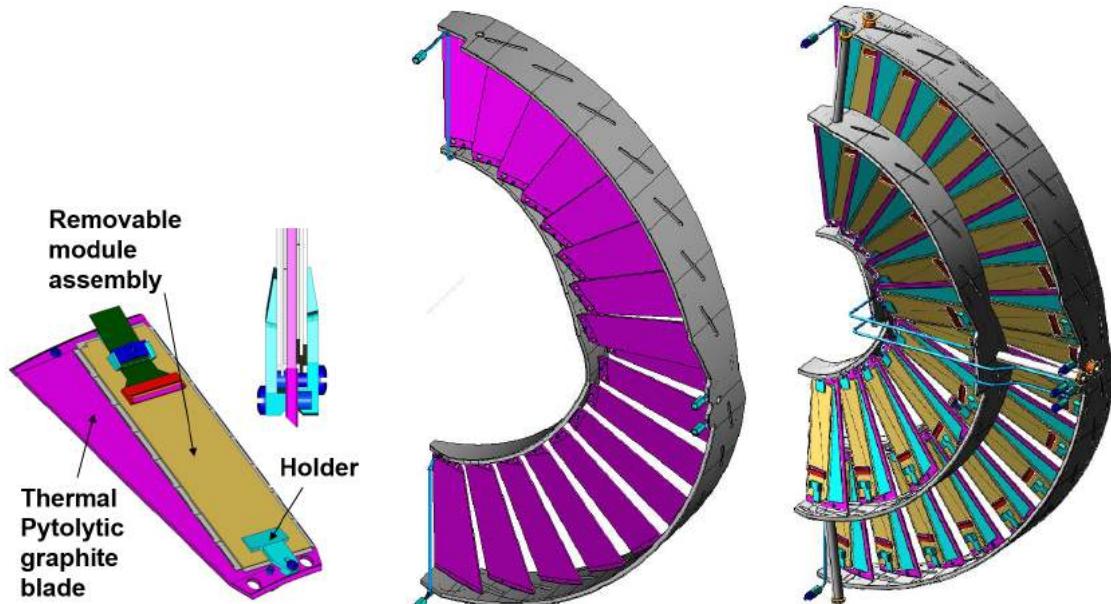
## 3378   **7.2 Phase 1 FPix upgrade**

3379       The Phase 1 upgraded FPix system is composed of three disks in each endcap, located  
 3380       at each end of the barrel detector, with a radial coverage ranging from 4.5 to 16.1

3381 cm. The first disk is located along the beam line at 29.1 cm from the IP; the second  
 3382 and third disks are located at 39.6 cm and 51.6 cm from the IP; each disk consists of  
 3383 two half disks. Some of the main features of the upgraded FPix System are:

- 3384     • Pixel size:  $100 \times 150 \mu\text{m}$
- 3385     • Only one type of modules: 2x8 ROC modules
- 3386     • Modules oriented radially to improve resolution in  $r - \phi$ .
- 3387     • Minimize the gap in 4-hit coverage between the end of the 4th-barrel layer and  
             the forward-most disk.
- 3389     • All three identical disks on each side of the IP.

3390     Figure 7.3 shows a schematic structure of the FPix half disk; each half disk is  
 3391 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).

3392 In total, there are 56 modules (896 ROCs) per half-disk, 34 modules in the outer  
 3393 ring and 22 modules in the inner ring. The pixel modules are attached to the blades  
 3394 by a pair of module holders. Modules are designed to be removable and replace-  
 3395 able without disassembling the half-disks; thus those modules that suffer failure or  
 3396 degradation can be easily replaced during an annual technical stop.

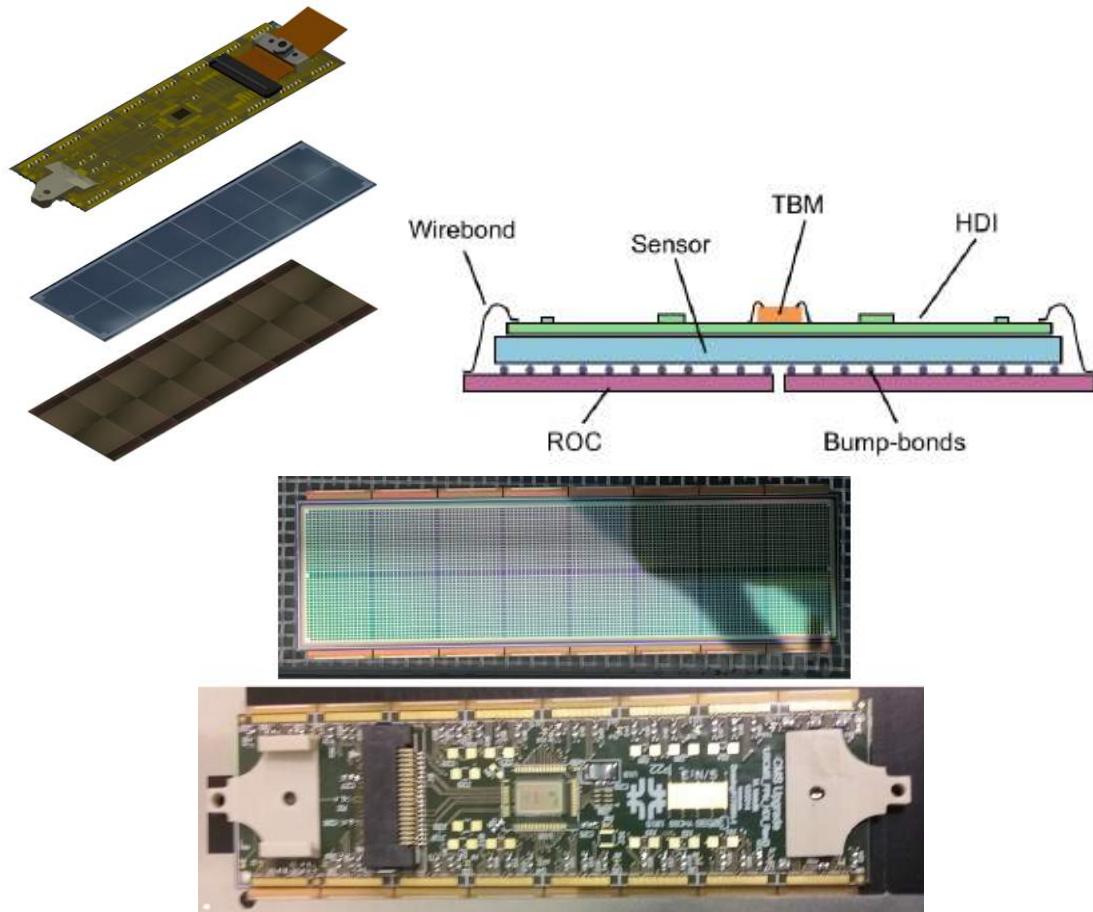
3397 Blades on the outer assembly are rotated by  $20^\circ$  forming a turbine-like geometry;  
 3398 in addition, they are arranged in an inverted cone array with the blades tilted by  $12^\circ$   
 3399 with respect to the IP in order to guarantee excellent resolution in both the azimuthal  
 3400 and radial directions throughout the FPIX acceptance angle for the inner assembly.

### 3401 **7.3 FPix module structure**

3402 The current CMS pixel detector is composed of 1184 pixel modules in the BPIX sector  
 3403 with a total 79 million of pixels; the FPix sector contains 672 with approximately 45  
 3404 million of pixels. Figure 7.4 shows an schematic view of the FPix modules structure.  
 3405 The  $n^+$ -in- $n$  *Silicon sensor* is Bump-Bonded to the 16 ROC to form the detector  
 3406 unit known as *Bump-Bonded Module* (BBM) with 66560 pixels. The *High Density*  
 3407 *Interconnect* (HDI) is glued on top of the BBM and wirebonded to the ROCs to  
 3408 provide them the required signals and power. The modules are attached to the  
 3409 support structure using the end holders glued to the HDI.

### 3410 **7.4 FPix module assembly**

3411 The construction of the modules for the current FPix system was divided between  
 3412 two sites located at Purdue University and UNL; testing facilities were located at  
 3413 University of Kansas and Fermi National Accelerator Laboratory (Fermilab). The

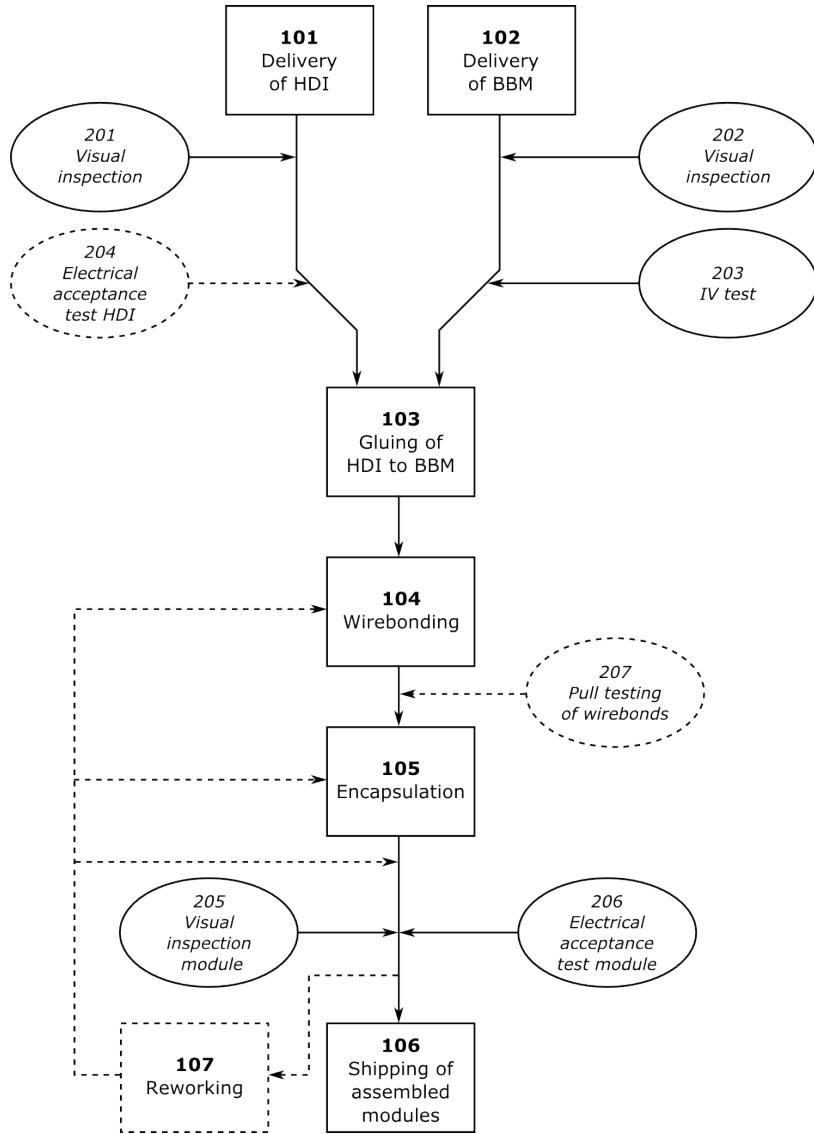


**Figure 7.4:** Top: FPix module structure; The bare silicon sensor is bump-bonded to the ROCs to form the BBM; then the HDI is glued on top of the BBM and wirebonded to the ROCs. Bottom: pictures of actual BBM and HDI.

3414 integration facility was based at Fermilab.

3415 The BBM was prepared by a commercial vendor, while the HDI was populated at  
 3416 Fermilab, with all the electronic components like resistors, capacitors and the central  
 3417 component known as *Token Bit Manager* (TBM) which is in charge of managing the  
 3418 information coming from the silicon sensors and going to the ROCs. Both BBM and  
 3419 HDI were sent to the assembly sites ready to be glued together.

3420 The module production procedure was designed following a production line struc-  
 3421 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.

3422 BBM and HDI arrive, they are submitted to visual inspection looking for defects,  
 3423 scratches, dents or short circuits. Modules passing the visual inspection are tested  
 3424 for electrical acceptance and performance. BBM and HDI are then glued employ-  
 3425 ing robotic pick-and-place machines that integrate optic tools, pattern recogni-  
 3426 tion algorithms, and glue dispensing; the semi-automated gluing process improves the

3427 uniformity of the technique. After 10 hours of curing, glued modules are moved to  
3428 the wirebonding station where ROCs and HDI are electrically connected employing  
3429 semi-automated ultrasonic wirebonding machines; occasionally, some of the wires are  
3430 pull tested for quality control. After this step, modules are fully functional, hence, a  
3431 basic functionality test is done at a subset of modules to control the manufacturing  
3432 process.

3433 In the next stage, the wirebonds are encapsulated with an elastomeric compound  
3434 (*Sylguard*) in order to protect them against mechanical damage and electrical shorts;  
3435 the encapsulation process is performed employing the robotic pick-and-place machine  
3436 which also integrates the encapsulant dispensing system. Once the encapsulation  
3437 ends, modules are mounted on module holders and submitted to a head cycle to cure  
3438 the sylguard.

3439 The module assembly sites were also responsible for the testing and characteriza-  
3440 tion of the assembled pixel modules. That testing included, visual inspection, elec-  
3441 trical acceptance, performance testing under controlled temperature conditions that  
3442 simulate the expected operational conditions; in case of any necessary reworking, the  
3443 modules were returned to the appropriate stage.

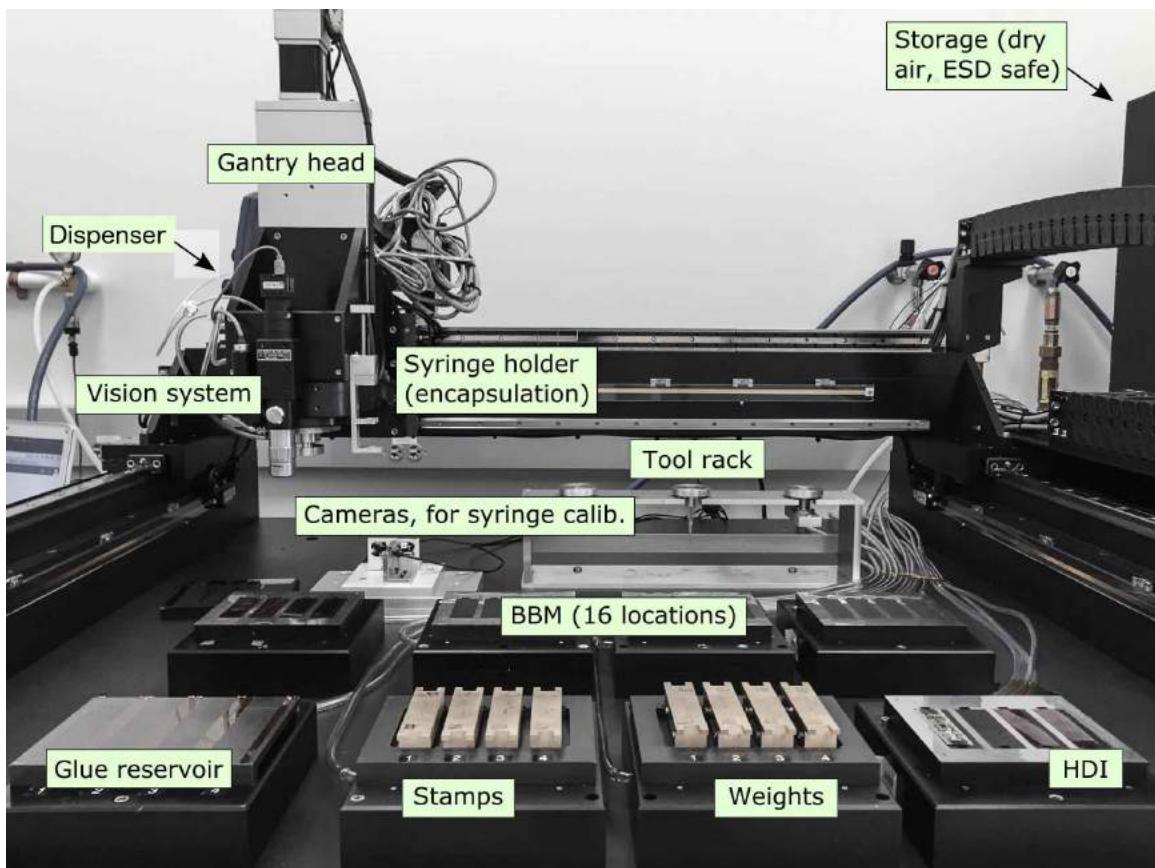
3444 In the final stage, the assembled and tested modules were shipped to University  
3445 of Kansas for further characterization.

3446 Each stage in the assembly procedure is documented with an *Standard Operat-*  
3447 *ing Procedure* (SOP) document that describes the procedures to be followed by the  
3448 operator. The full set of SOPs can be found in Reference [160].

3449 In the following sections a detailed description of the gluing and encapsulation  
3450 stages will be presented.

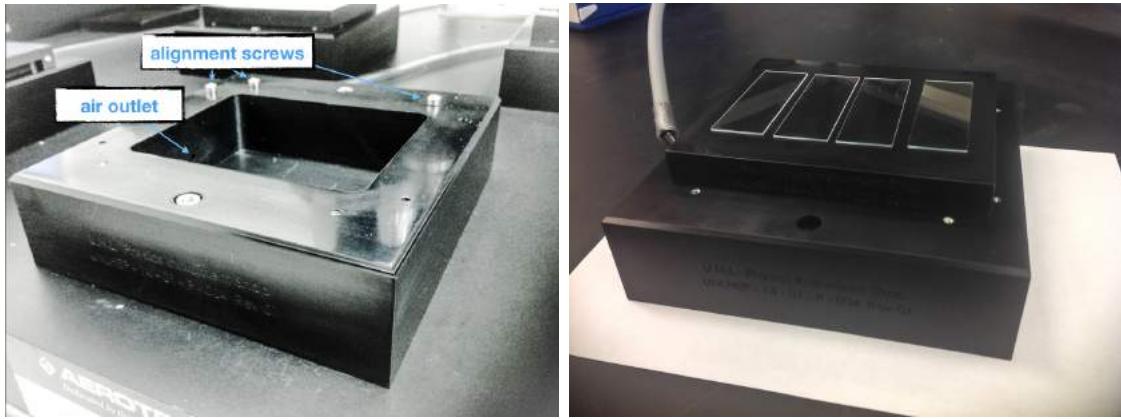
### 3451 7.4.1 Pick and place machine setup

3452 Figure 7.6 shows the full setup used to perform the gluing and encapsulation steps.  
 3453 The gantry used in the setup is a custom made *AGS15000 Series Gantry*, fabricated  
 3454 by Aerotech [161], which offers translational motion in 3D ensuring coverage of any  
 3455 position in the work field; in addition, rotational motion is provided in the *gantry*  
 3456 *head* in the usual x-y plane (gantry table plane).



**Figure 7.6:** Full gluing and encapsulation setup.

3457 A set of eight hard-anodized aluminum chucks, composed of a *base chuck* and a  
 3458 *plate chuck* each, henceforth chuck and plate respectively, were designed to house the  
 3459 parts and tools needed along the gluing process; Figure 7.7 shows the details of a  
 3460 chuck.



**Figure 7.7:** Left: Chuck detailed internal view. Right: full chuck housing glass slides. The vacuum connection is visible on the left.

3461        Each chuck is connected to an independent vacuum line such that the plate is  
 3462   hold fixed; both pieces are polished to seal the vacuum with no use of O-rings. The  
 3463   three screws serves as references for aligning the plates with the chucks. There are  
 3464   four types of plates; HDI/BBM plate, the glue reservoir plate, stamp plate, weight  
 3465   plate.

### 3466    Chucks

3467   Four chucks are used to accommodate sixteen BBMs (four per plate); the holes in  
 3468   the BBM/HDI plate (see Figure 7.8) are intended to hold the BBM/HDI safely fixed  
 3469   to the plate by the action of the vacuum, while the stencil (100  $\mu\text{m}$  in thickness)  
 3470   allows for a very accurate positioning of the BBM/HDI; it is thin enough so that the  
 3471   alignment is controlled by the edges of the ROC and no force is applied to the sensor.

3472        One chuck is dedicated to accommodate four HDIs. Although BBM/HDI plates  
 3473   have the same design, the HDI chuck have four independent pockets instead of only  
 3474   a big one, in order to enable the release of one HDI at a time; hence, it is connected  
 3475   to 4 vacuum lines. That is not required for the BBMs because they are no moved  
 3476   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.

3477 response to the HDI back surface which is not totally flat but has irregularities; these  
 3478 irregularities caused vacuum leaks that were addressed by adding a kapton tape layer  
 3479 to the HDI plate, as shown in the center of Figure 7.8. The tracks ensure the vacuum  
 3480 action and the tape flexibility ensures the sealing.

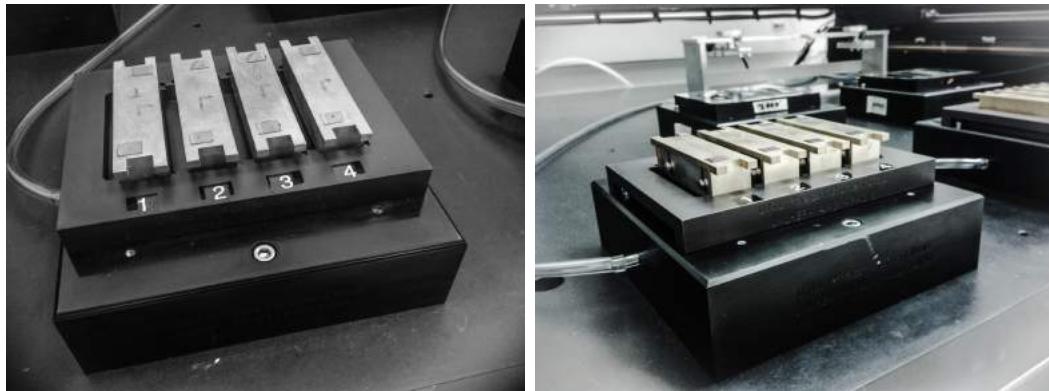
3481 One chucks holds the *glue reservoir* plate, as shown in Figure 7.9. Each of the  
 3482 four reservoirs is a pocket just 100  $\mu\text{m}$  deep, suitable for retaining sufficient glue to  
 3483 be applied to the BBM.



**Figure 7.9:** Glue reservoir plate. The four pockets are 100  $\mu\text{m}$  deep.

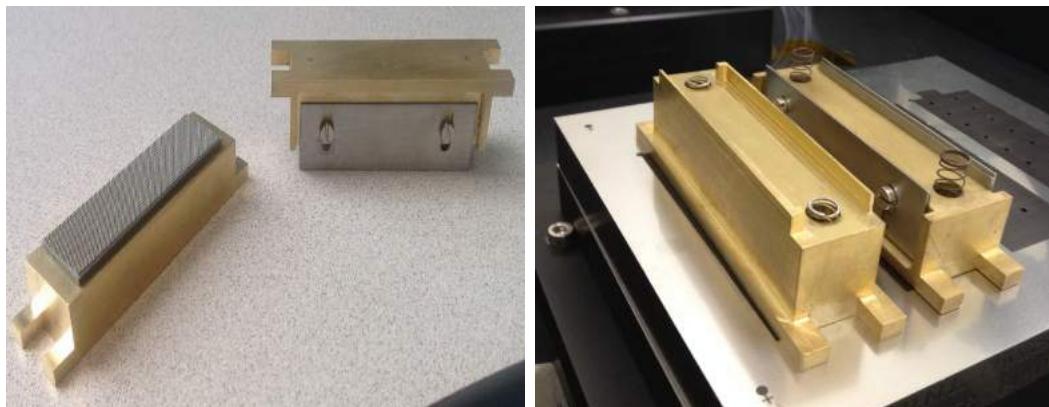
3484 The remaining two chucks house the *stamp plate* and the *weight plate* which in

3485 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).

3486 **Stamp and weight tools**

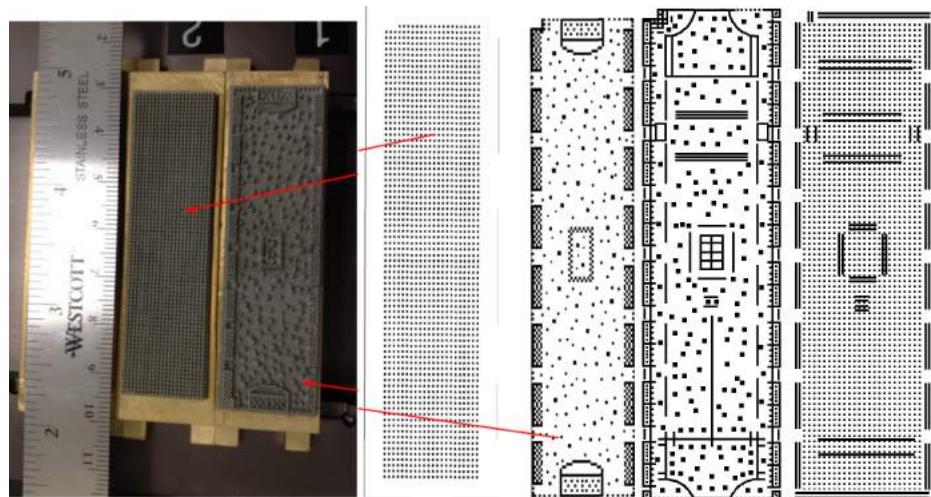


**Figure 7.11:** Stamp and weight tools. Both tools are made of brass; the stamp tool includes a rubber stamp while the weight tool includes four stainless steel blades to apply force while curing. The final weight tool design eliminates the blades (right).

3487 Stamp and weight tools are a set of custom made tools, all produced by the UNL  
 3488 Physics department machine shop (see Figure 7.11). The very first design of the  
 3489 weight tool included four stainless steel blades and two springs; the blades matched  
 3490 the rows of 8 ROC bond pads on the HDI to apply force while curing. The springs  
 3491 apply force to the module end holders on the HDI. The final design of the tool

3492 eliminates the issues associated to the alignment of the blades, by integrating them  
 3493 into the design in the form of narrow blade-like brass edges. The weight tools are  
 3494 made with 260 g of brass.

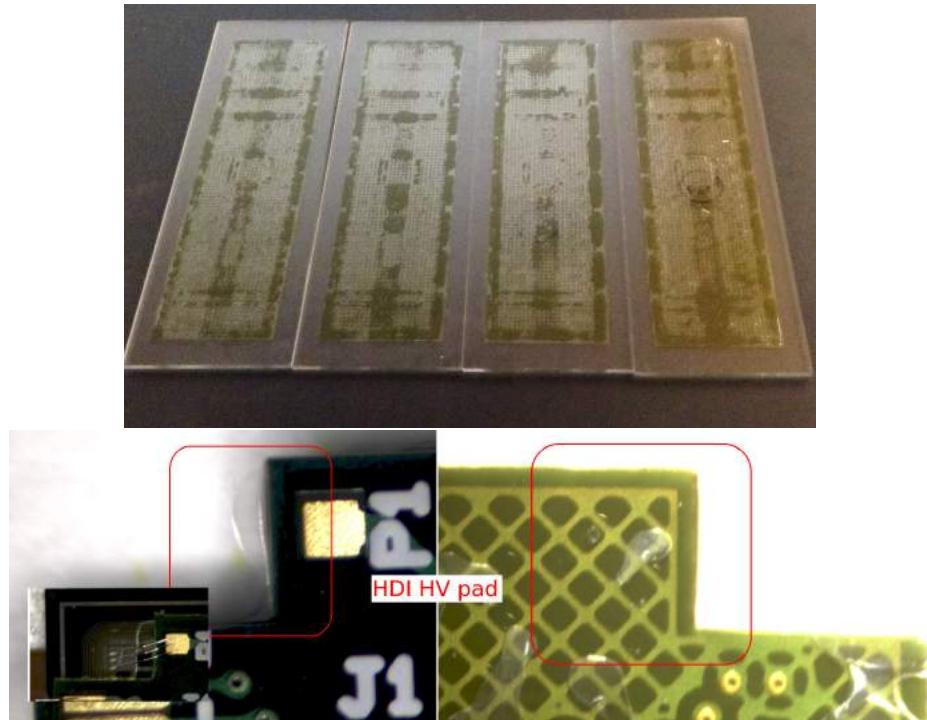
3495 The stamp tool is composed of a brass piece of 200 g and a rubber stamp piece  
 3496 attached to the bottom side of the brass piece; it is used to pick the glue from the glue  
 3497 reservoir and then stamp it over the BBM. An extensive testing process was performed  
 3498 in order to determine the most appropriate features of the gluing strategy. Figure 7.15  
 3499 shows the four stamp patterns tested and a picture of the first two attached to the  
 3500 stamp tools; the variations in the pattern design were based on the results from testing  
 3501 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.

3502 • the size of contact area, and in particular the support given to the edges of the  
 3503 HDI where the bond pads and the high-voltage (HV) pad are located. This is a  
 3504 critical aspect, given that the wirebonding relies on the steadiness of the pads  
 3505 to be connected.

3506     • the amount of glue dispensed, and in particular the glue spreading out of the  
 3507       HDI area. An excess of glue, scattered beyond the HDI edge would go between  
 3508       the ROC and the sensor, affecting the functionality of the bump bonds connect-  
 3509       ing them; in the case of the HV pad, it was observed that excess of glue covered  
 3510       the pad on the sensor, making impossible to wire it. Figure 7.13 shows pictures  
 3511       of a glue test using the final stamp pattern. Note The support that it provides  
 3512       to the HDI bond pads and the HV pad and the almost null glue spreading out,  
 3513       which justify why it was chosen.



**Figure 7.13:** 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.

3514     • the dipping time of the stamp tool in the glue reservoir.  
 3515     • depth of the glue reservoir

3516 **Vision system**

3517 A vision system, attached to the gantry head, is used to locate the module components  
3518 and tools employed in the assembly process. It is composed of a HD industrial digital  
3519 camera and a lens system, mitutoyo Wide-field Video Microscope Unit WIDE VMU

3520 **Tool rack**

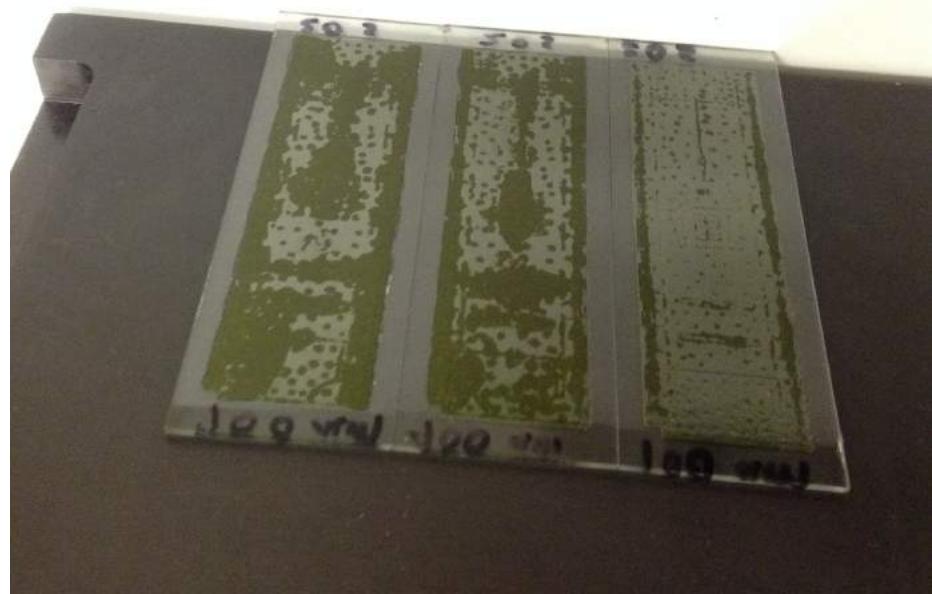
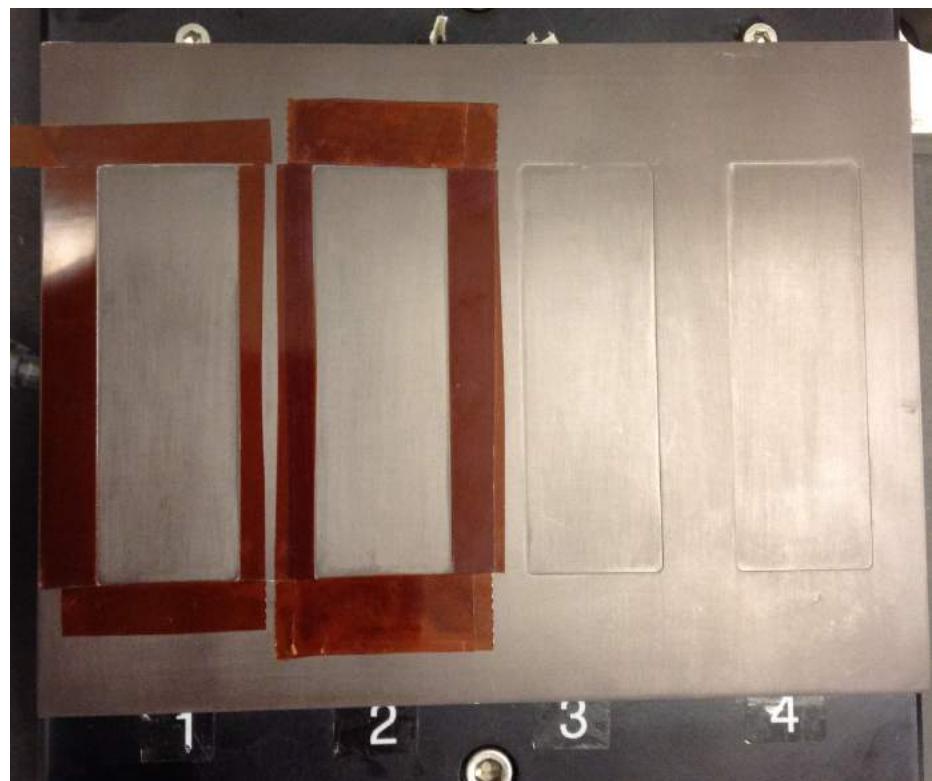
3521 The module gluing sequence begins by manually placing pre-tested, BBMs and HDI  
3522 on vacuum chucks on the baseplate of the pick-and-place machine.

3523 The machine program successively moves the camera (fixed to the machine motion  
3524 head) to view the fiducial on the BBM sensors and HDI components and acquires  
3525 the fiducial location using pattern recognition, picks up a dispensing tool from a the  
3526 tool rack and dispenses epoxy on the sensors, returns the dispensing tool to the tool  
3527 rack, picks up a vacuum tool from the tool rack to pick-and-place individual HDI  
3528 onto sensors (making adjustments based on the actual part locations in the machine  
3529 to accurately align and join the components), and returns the vacuum tool to the tool  
3530 rack. Module end holders are also aligned and glued to the modules using custom  
3531 tooling and the pick-and-place machine. Following mechanical assembly, HDI are  
3532 wirebonded to the ROCs using semi-automated ul- trasonic wirebonding machines.  
3533 Routine pull tests of sample wirebonds will be performed for quality control. The  
3534 wirebonds will be encapsulated with an elastomeric compound using semi-automated  
3535 dispensing equipment. The module assembly sites will also be responsible for the  
3536 testing and characterization of the assembled pixel modules. Modules will be ther-  
3537 mally cycled within the operating temperature range (-20 °C to 20 °C) while  
3538 monitoring ROC digital and analog currents. Modules which pass the acceptance  
3539 criteria will then be assembled onto the half-disk blades.

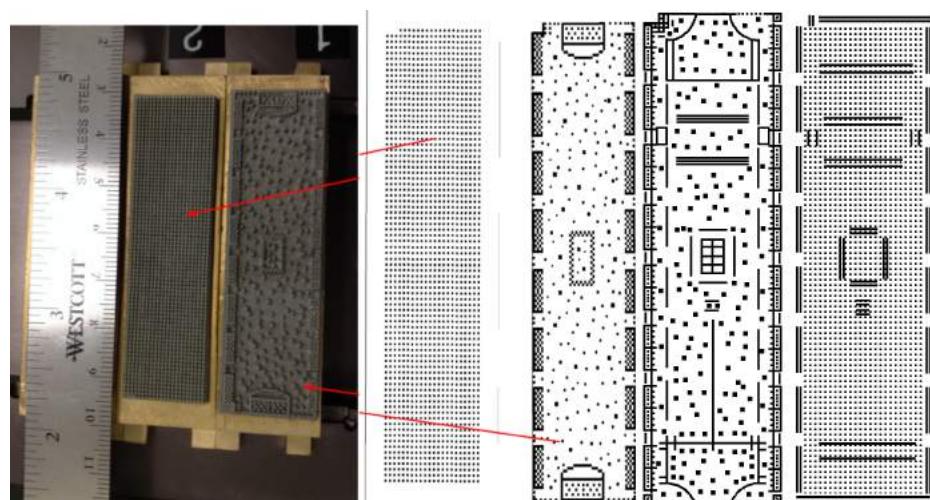
3540        The module assembly and testing schedule will depend on the throughput of the  
3541        pixel modules delivered from the bump-bonding vendors to the module assembly sites.

3542        **7.4.2     The Encapsulation stage**

3543        **7.4.3     The FPix module production yields**



**Figure 7.14:** 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.



**Figure 7.15:** 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.

<sup>3544</sup> **Appendix A**

<sup>3545</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

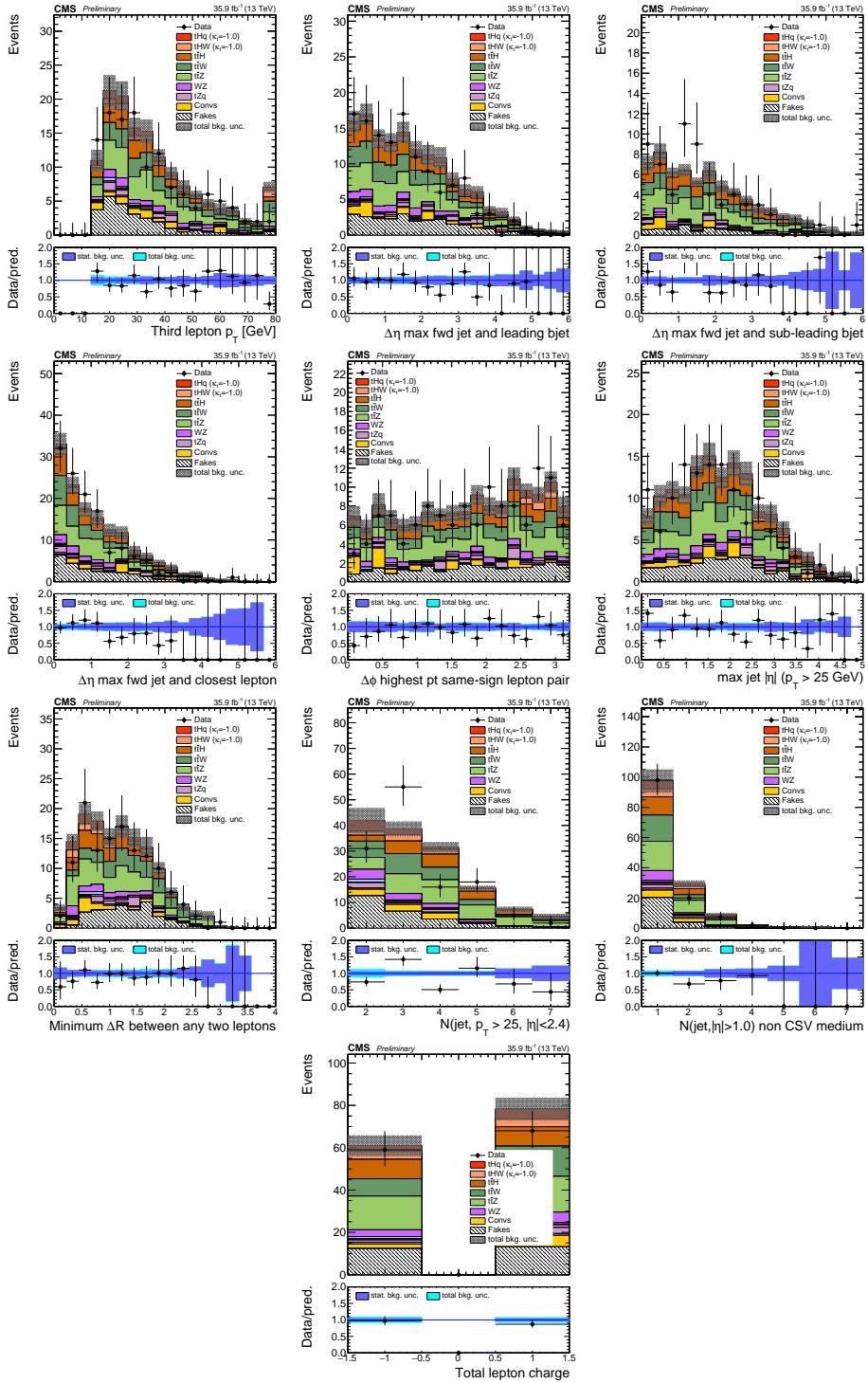
**Table A.4:** List of background samples used in this analysis (CMSSW 80X). The first section of the table lists the samples used in simulation to extract the final yields and shapes; the second section lists the samples of the processes for which the yields are estimated from data. The MC simulation 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>3546</sup> **Appendix B**

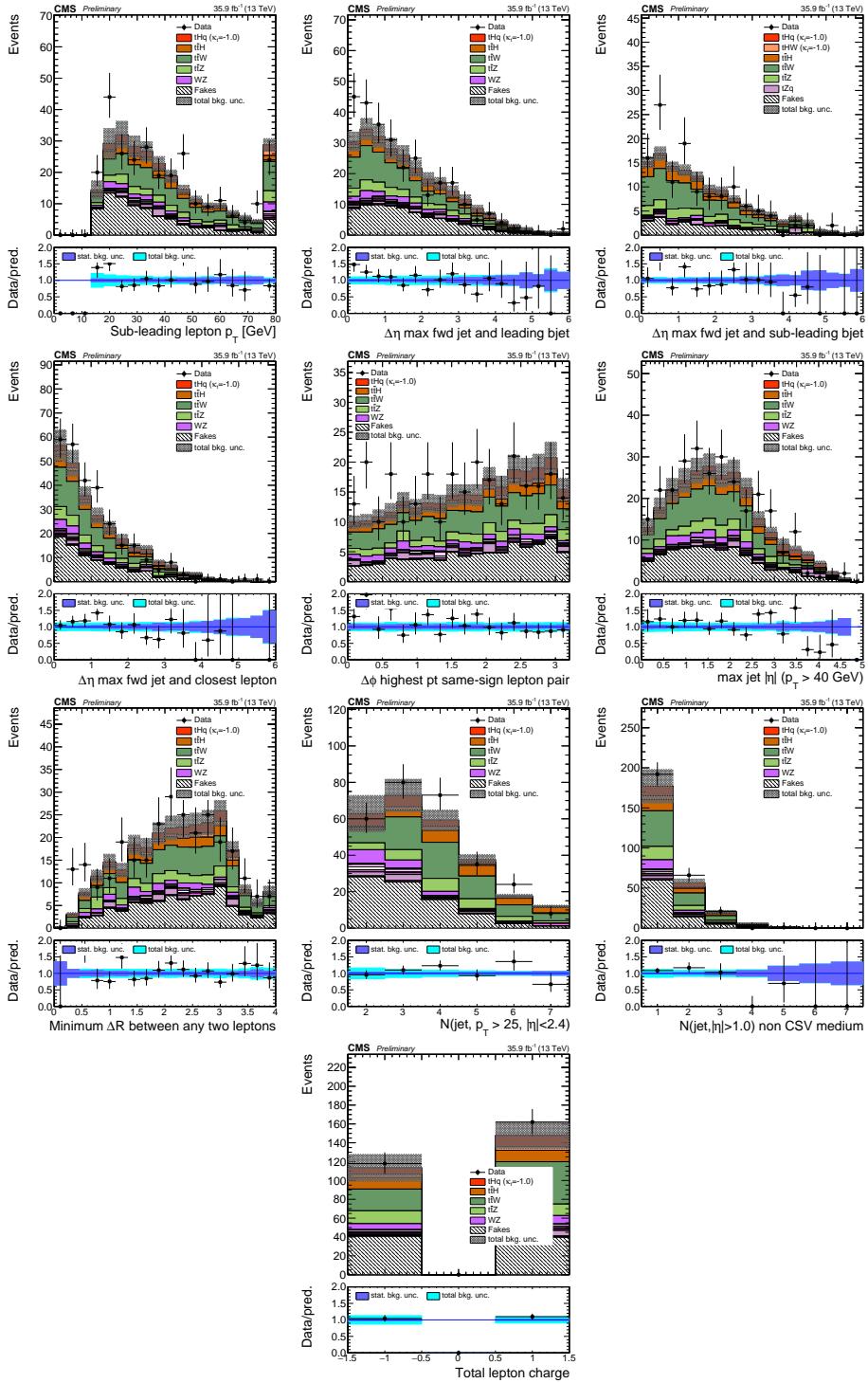
<sup>3547</sup> **Aditional plots**

<sup>3548</sup> **B.1 Pre-selection kinematic variables**

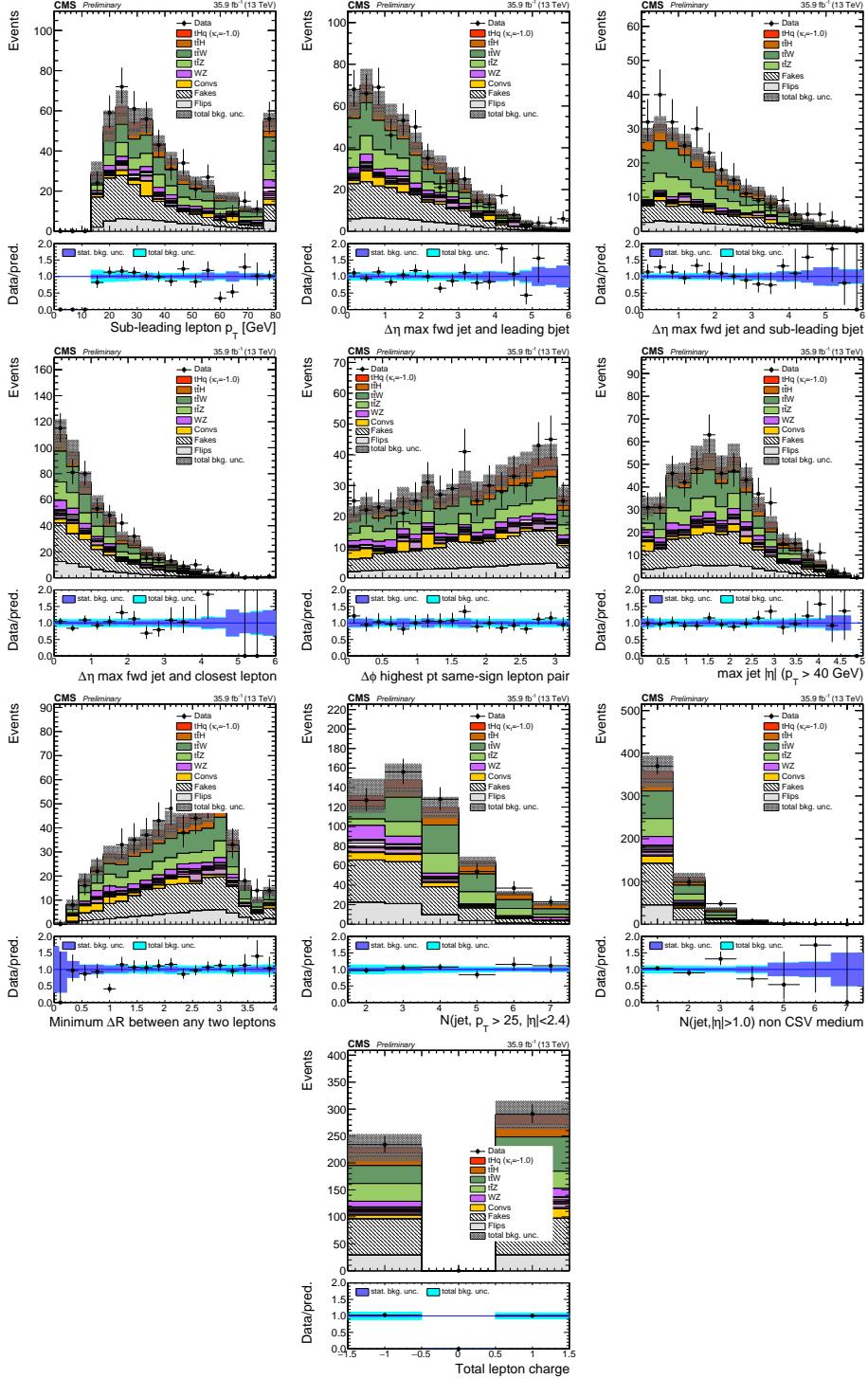
<sup>3549</sup> Figures B.1, B.2 and B.3 show the distributions of some relevant kinematic variables,  
<sup>3550</sup> normalized to the cross section of the respective processes and to the integrated  
<sup>3551</sup> luminosity.



**Figure B.1:** Distributions of input variables to the BDT for signal discrimination, three lepton channel, normalized to their cross section and to  $35.9 \text{ fb}^{-1}$ .

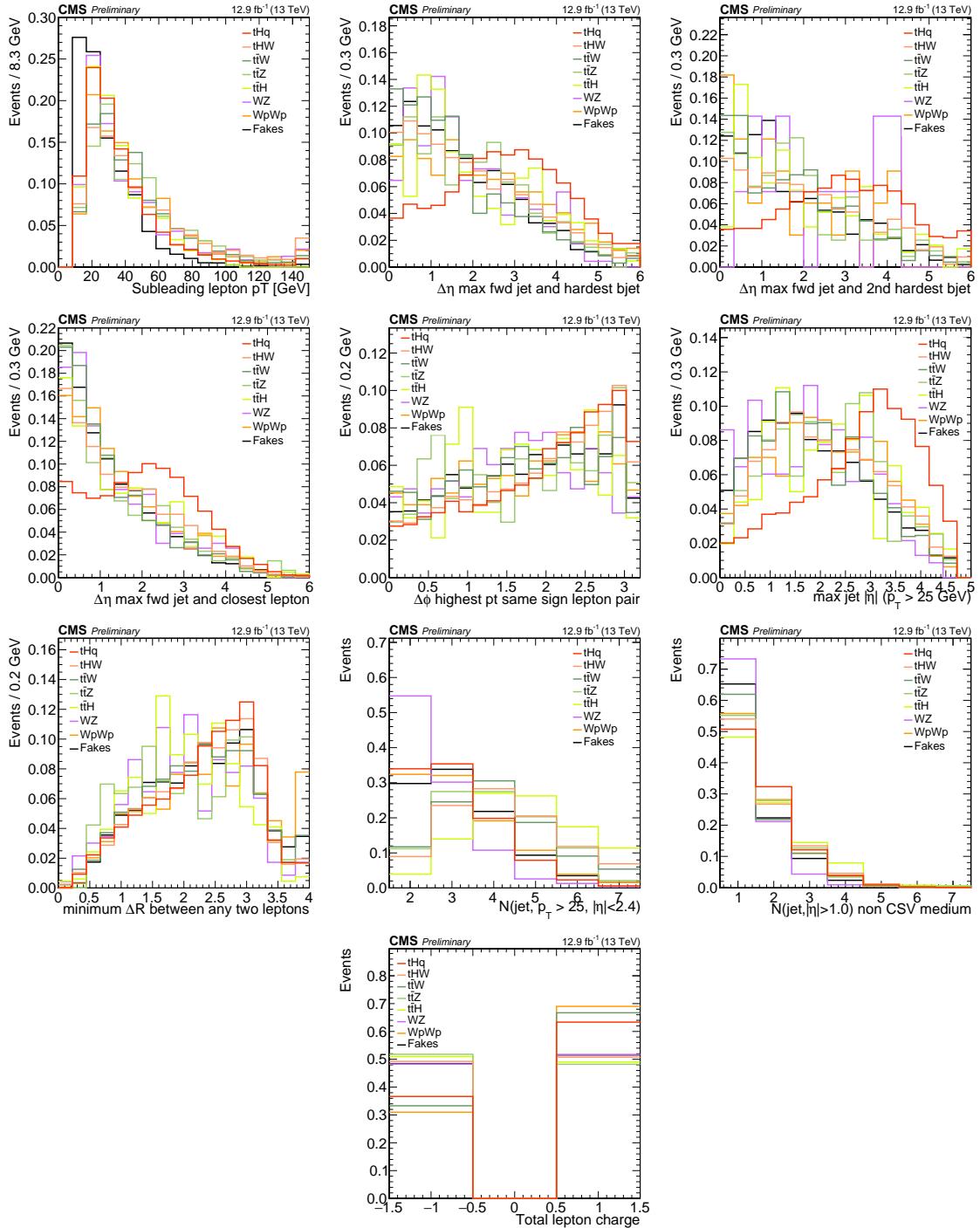


**Figure B.2:** Distributions of input variables to the BDT for signal discrimination, in  $\mu^\pm \mu^\pm$  channel, normalized to their cross section and to  $35.9 \text{ fb}^{-1}$ .



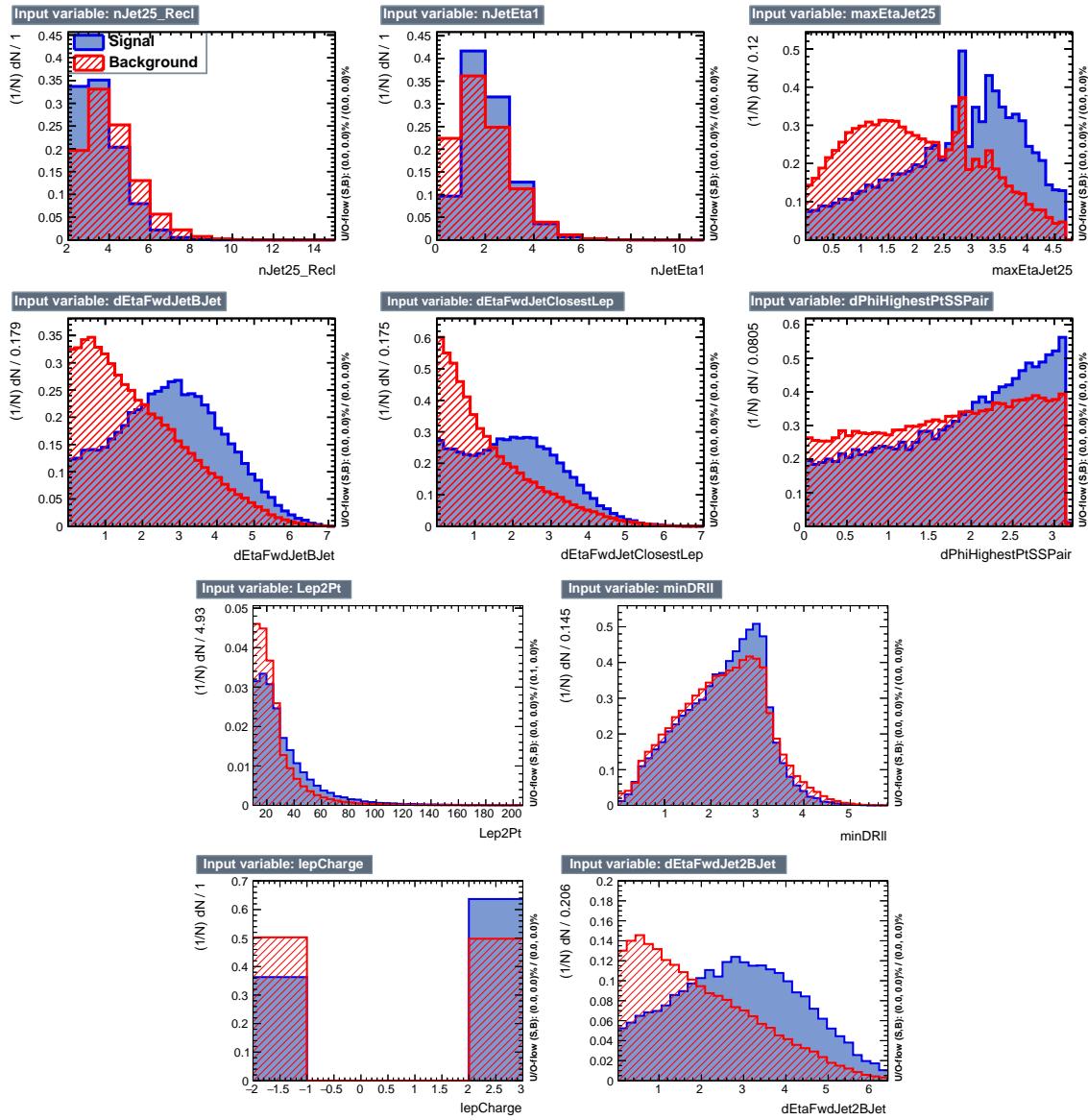
**Figure B.3:** Distributions of input variables to the BDT for signal discrimination, in  $e^\pm\mu^\pm$  channel, normalized to their cross section and to  $35.9\text{fb}^{-1}$ .

3552 B.2 BDTG input variables for  $2lss$  channel

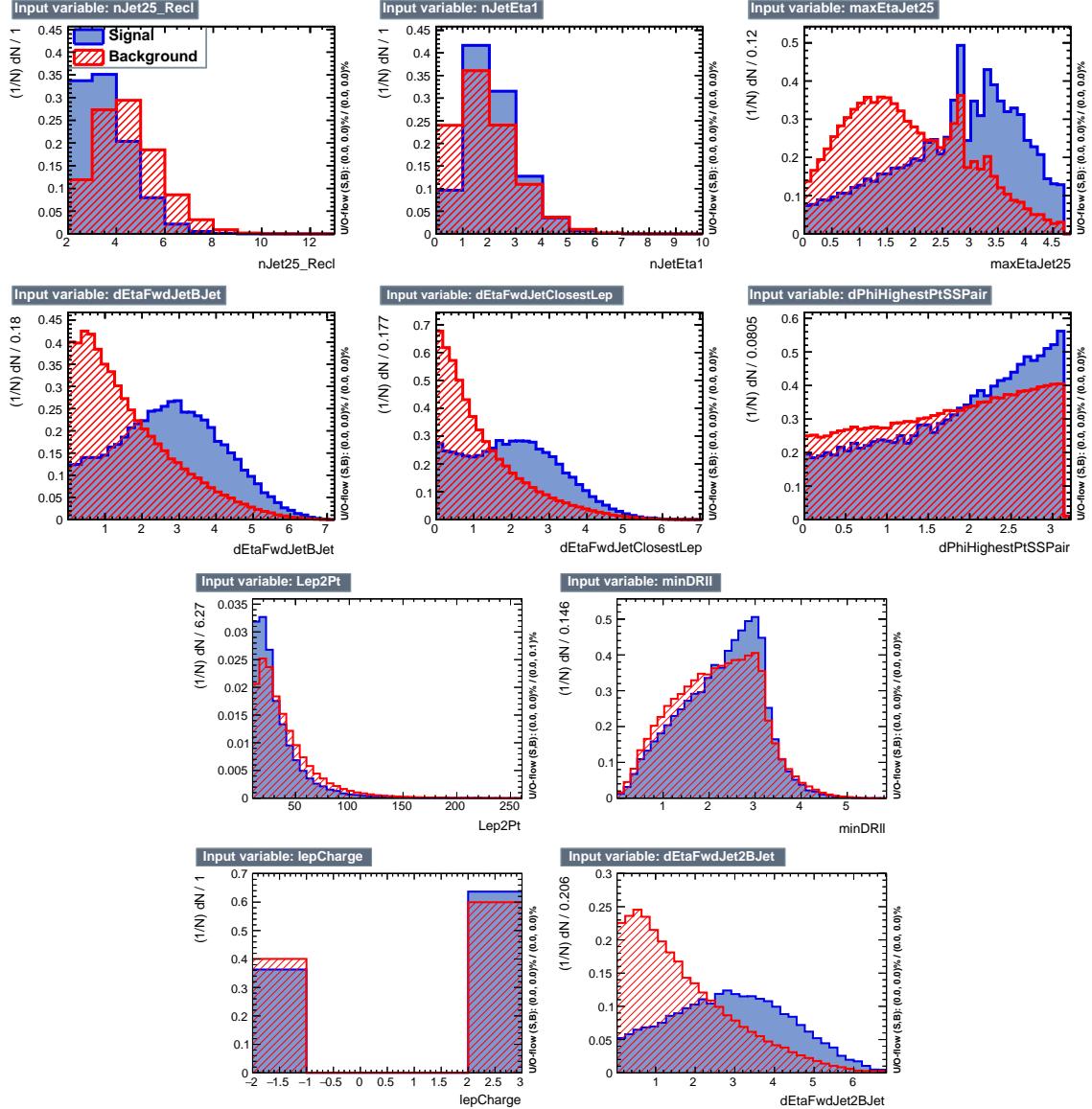


**Figure B.4:** Distributions of input variables to the BDT for signal discrimination, two lepton same sign channel.

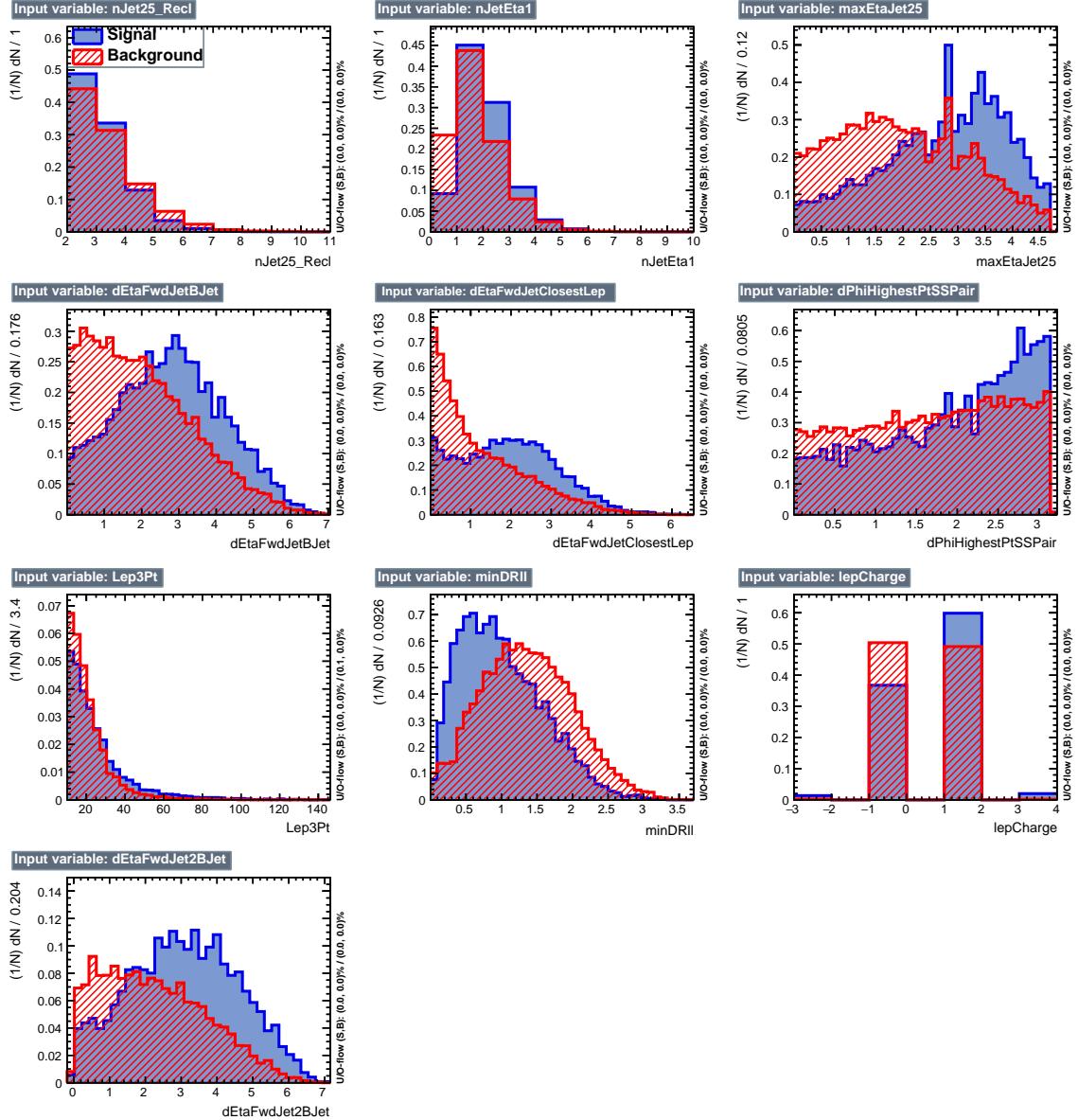
3553 **B.3 Input variables distributions from BDTG**  
 3554 classifiers



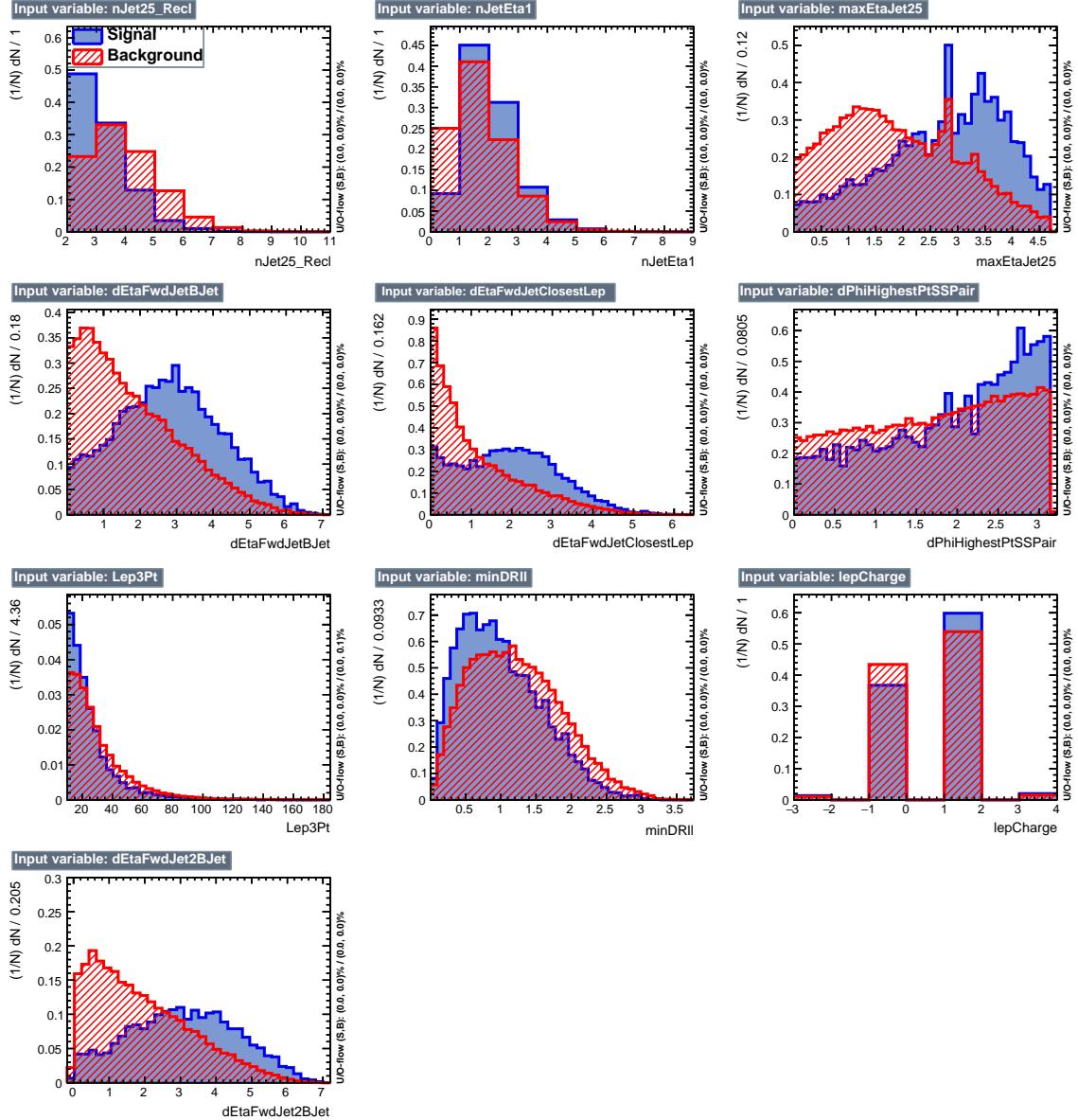
**Figure B.5:** BDT input variables as seen by BDTG classifier for the  $2lss$  channel,  $tHq$  signal (blue) discriminated against  $t\bar{t}$  background (red).



**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).

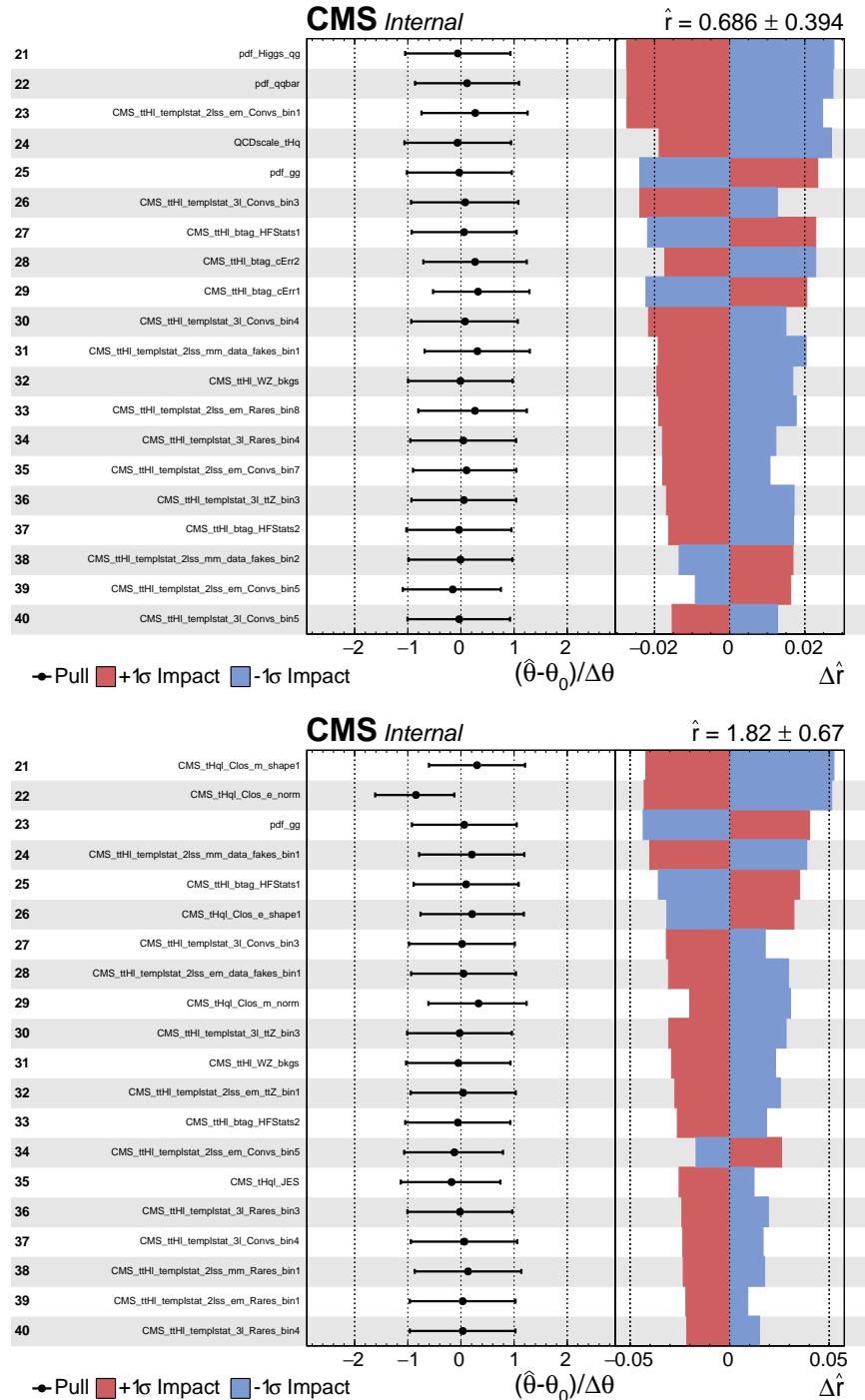


**Figure B.7:** BDT input variables as seen by BDTG classifier for the  $3l$  channel,  $tHq$  signal (blue) discriminated against  $t\bar{t}$  background (red).

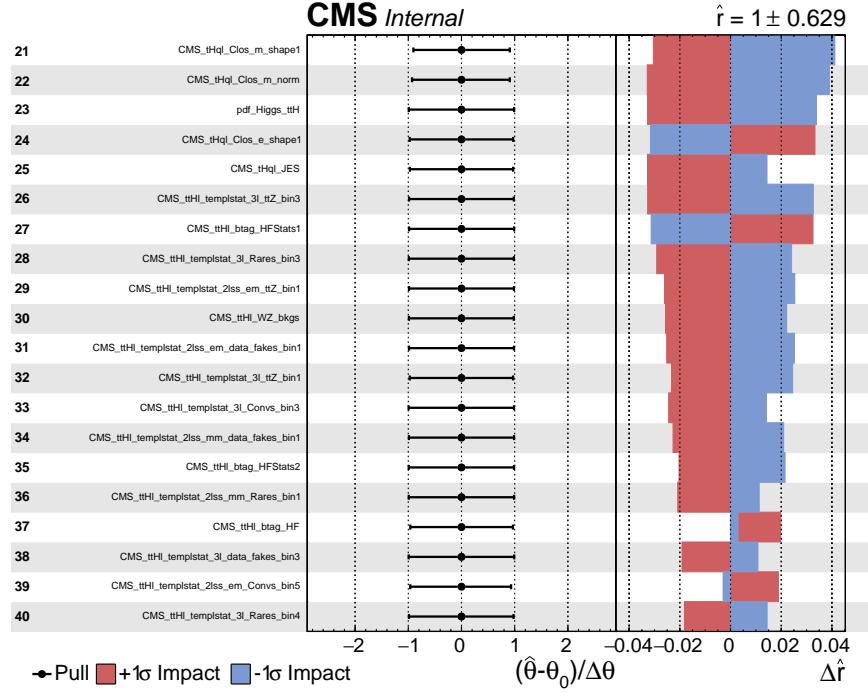


**Figure B.8:** BDT input variables as seen by BDTG classifier for the  $3l$  channel,  $tHq$  signal (blue) discriminated against  $t\bar{t}V$  background (red).

3555 **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.

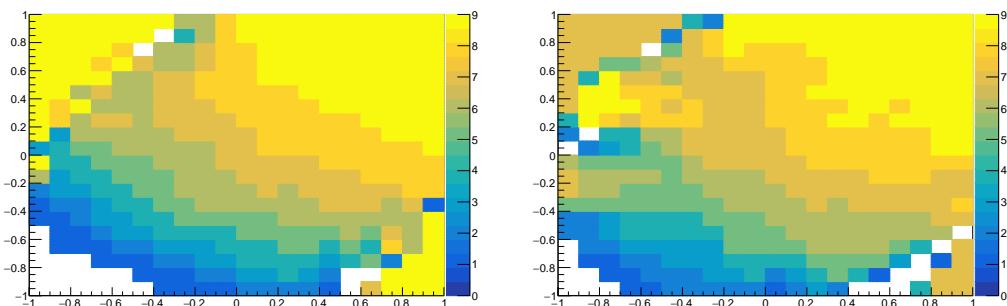
3556 **Appendix C**

3557 **Other binning strategies**

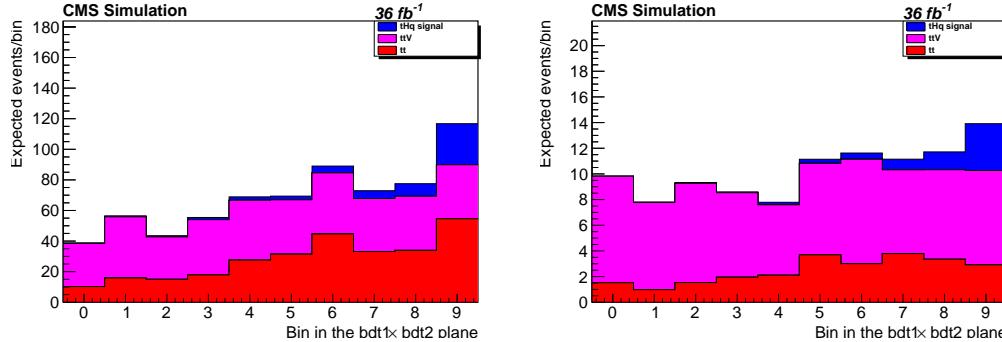
3558 Two additional strategies of clustering regions in the 2D plane of  $BDTG_{tt}$  vs  $BDTG_{ttV}$   
 3559 into bins were attempted, following studies done and documented in great detail in  
 3560 Reference [149]. A brief description is provided in the following.

3561 **Clustering by S/B ratio**

3562 In this method, the 2D plane is clustered into a given number of bins corresponding  
 3563 to regions where S/B is within a certain range. The bin borders are determined  
 3564 such that the number of background events in each bin is approximately equal. The  
 3565 resulting regions for  $2lss$  and  $3l$  events are shown in Figure C.1, while the expected  
 3566 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).



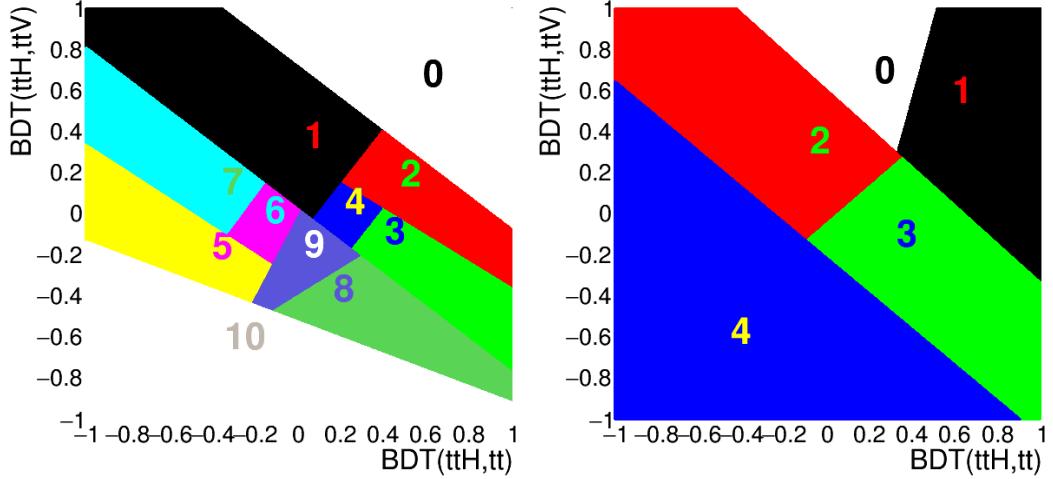
**Figure C.2:** Final bins (corresponding to S/B regions in the 2D plane) for  $2lss$  and  $3l$  (right).

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.

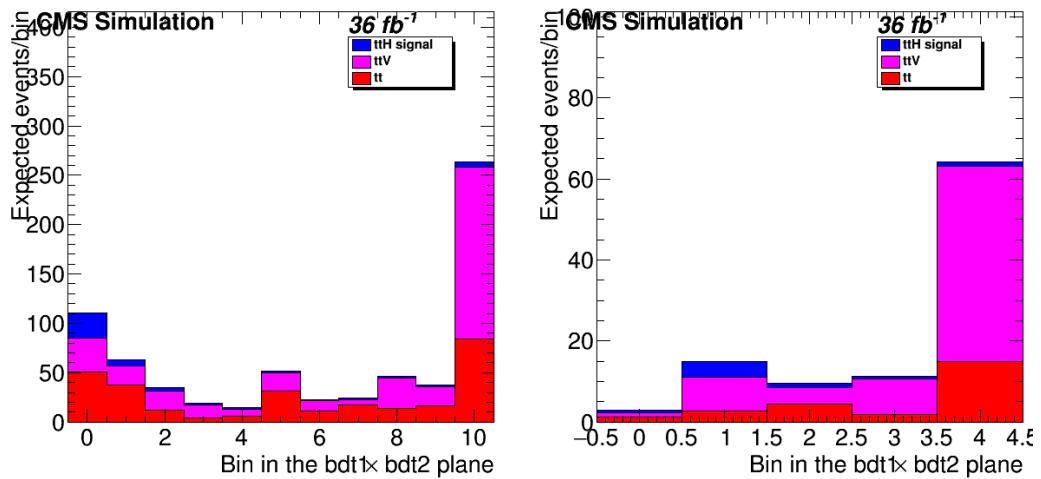
#### ***k*-Means geometric clustering**

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).

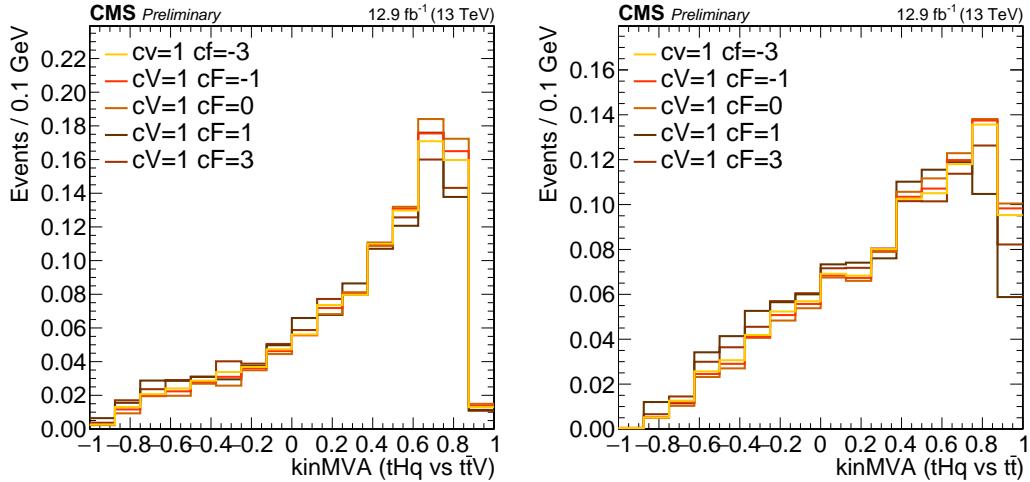


**Figure C.4:** Final bins using a  $k$ -means algorithm for  $2lss$  (left) and  $3l$  (right). Note that the bin numbering here is such that signal-like bins are lower.

3579 **Appendix D**

3580 **BDTG output variation with  $\kappa_V/\kappa_t$**

3581 The BDTG classifier output was described in Section in the  $\kappa_t = -1, \kappa_V = 1$  scenario; the  
 3582 change of BDTG classifiers output shape when varying the  $\kappa_V/\kappa_t$  coupling scenario  
 3583 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).

3584

3585 Given that the BDT classifier output shape does not change, it is enough to train  
 3586 the BDTG in one of the  $\kappa_t/\kappa_V$  points. It was chosen the SM point.

<sup>3587</sup> **Appendix E**

<sup>3588</sup>  **$tHq$ - $t\bar{t}H$  overlap**

<sup>3589</sup> This section provides a quick overview of the differences and commonalities in event  
<sup>3590</sup> selections between this analysis and the  $t\bar{t}H$  multilepton search [149]. The object  
<sup>3591</sup> selections of the two analysis are perfectly synchronized due to shared frameworks  
<sup>3592</sup> and samples. The only exception is the usage of forward jets ( $|\eta| > 2.4, p_T > 40$  GeV)  
<sup>3593</sup> in this analysis. Such jets are not considered in the  $t\bar{t}H$  analysis.

<sup>3594</sup> Table E.1 gives an overview of the main differences in the event selections. Here,  
<sup>3595</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>3596</sup> analysis are jets that do not pass the CSV loose working point and are either central  
<sup>3597</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>3598</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.

3599       Table E.2 shows the total events yields in the individual channels, and the yield  
 3600 of shared events between each channel, for the  $tHq$  signal sample, the  $t\bar{t}H$  signal  
 3601 sample, and the data. In the data, for the  $3l$  channel, about 80% of events passing  
 3602 the  $tHq$  selection also pass the  $t\bar{t}H$  selection, constituting about 70% of that channel.  
 3603 In the  $2lss$  channel, about 50% of data events passing the  $tHq$  selection also pass the  
 3604  $t\bar{t}H$  selection, but these events constitute almost 90% of the  $t\bar{t}H$  selection in those  
 3605 channels. Similar overlaps are also seen in the  $tHq$  and  $t\bar{t}H$  signal samples.

3606       There is no migration between different channels and different selections, i.e., no  
 3607 events passing the selection of a given  $tHq$  channel pass the selection of any other  
 3608 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

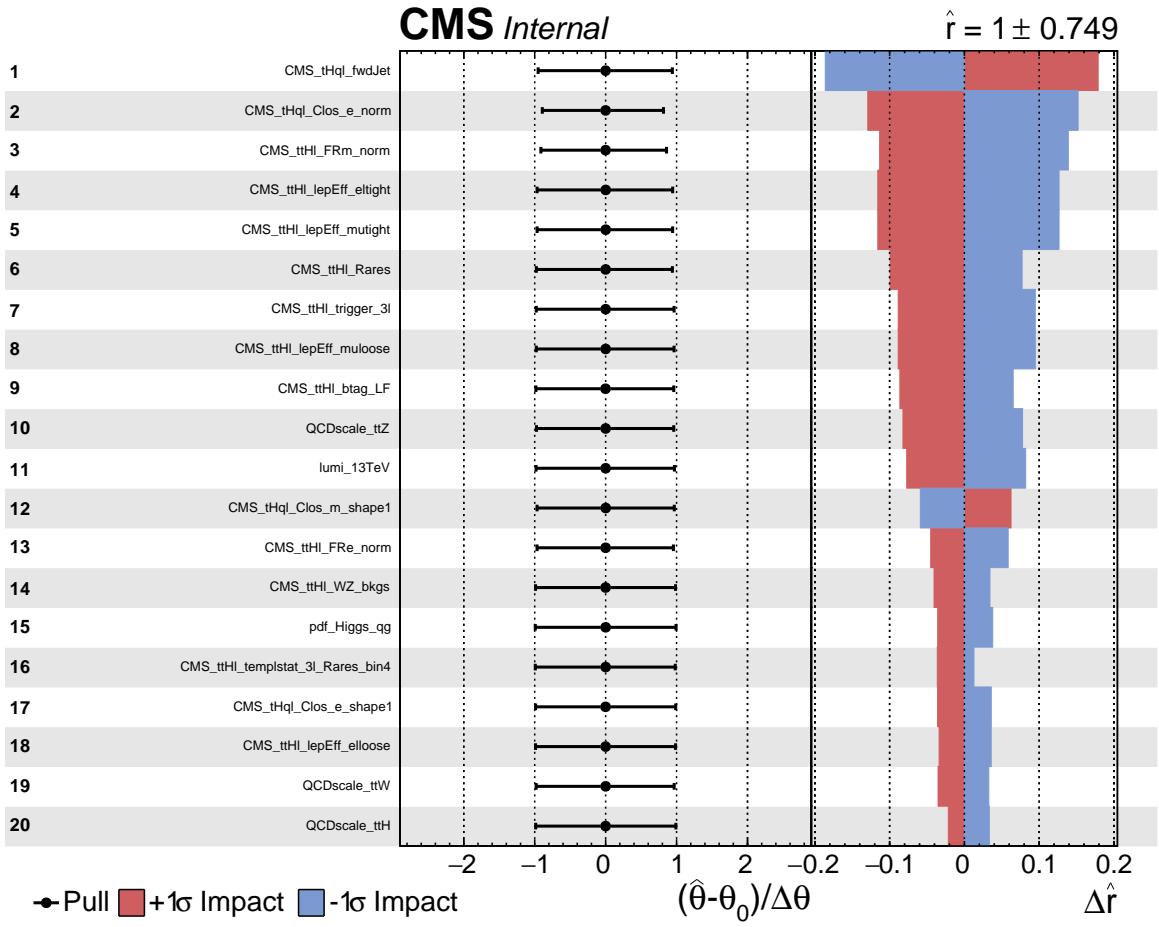
Data	$tHq$	$t\bar{t}H$	Common	(% $tHq$ )	(% $t\bar{t}H$ )
$\mu^\pm\mu^\pm$	280	160	140	50.0	87.5
$e^\pm\mu^\pm$	525	280	242	46.1	86.4
$e^\pm e^\pm$	208	90	79	38.0	87.8
$\ell\ell\ell$	126	154	104	82.5	67.5

**Table E.2:** Individual and shared event yields between this analysis ( $tHq$ ) and  $t\bar{t}H$  multilepton selections.

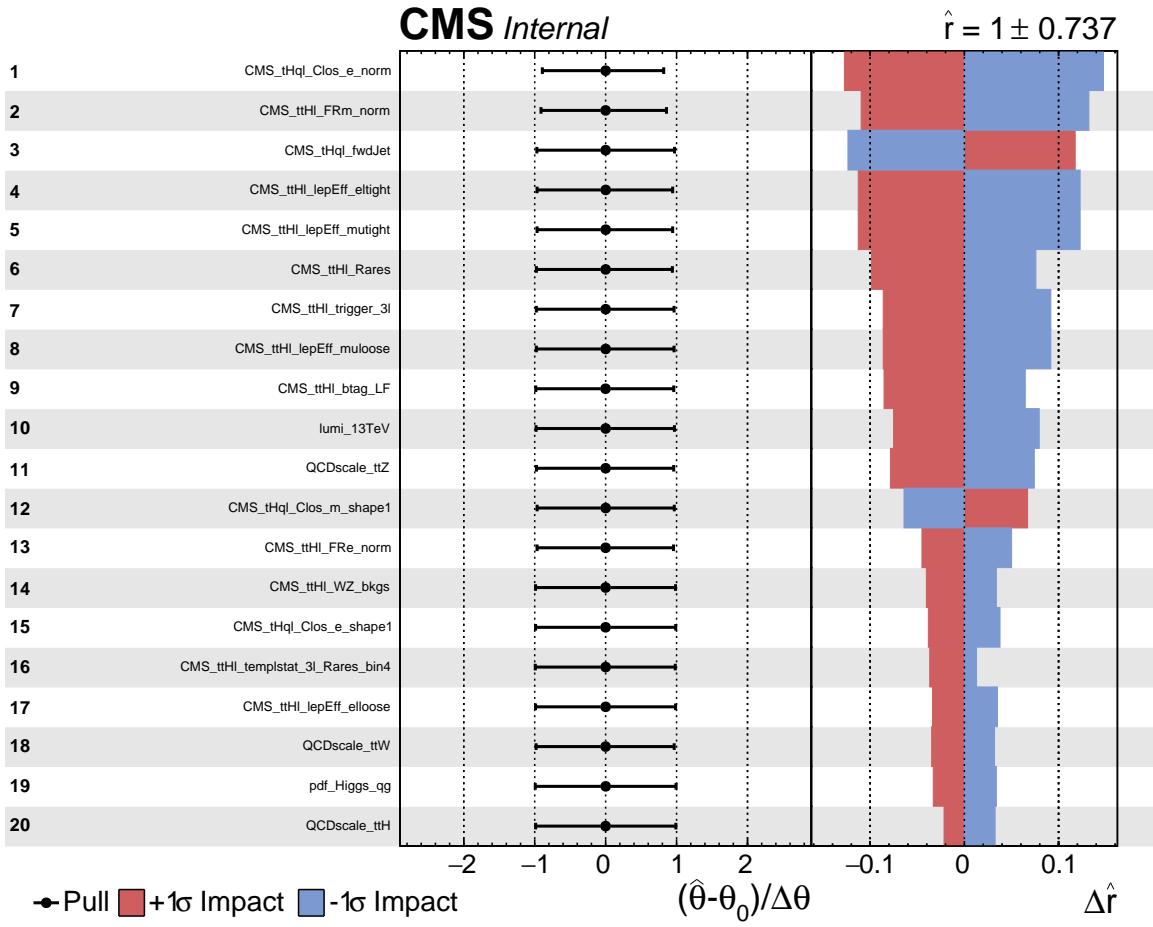
3609 **Appendix F**

3610 **Forward jet impact plots**

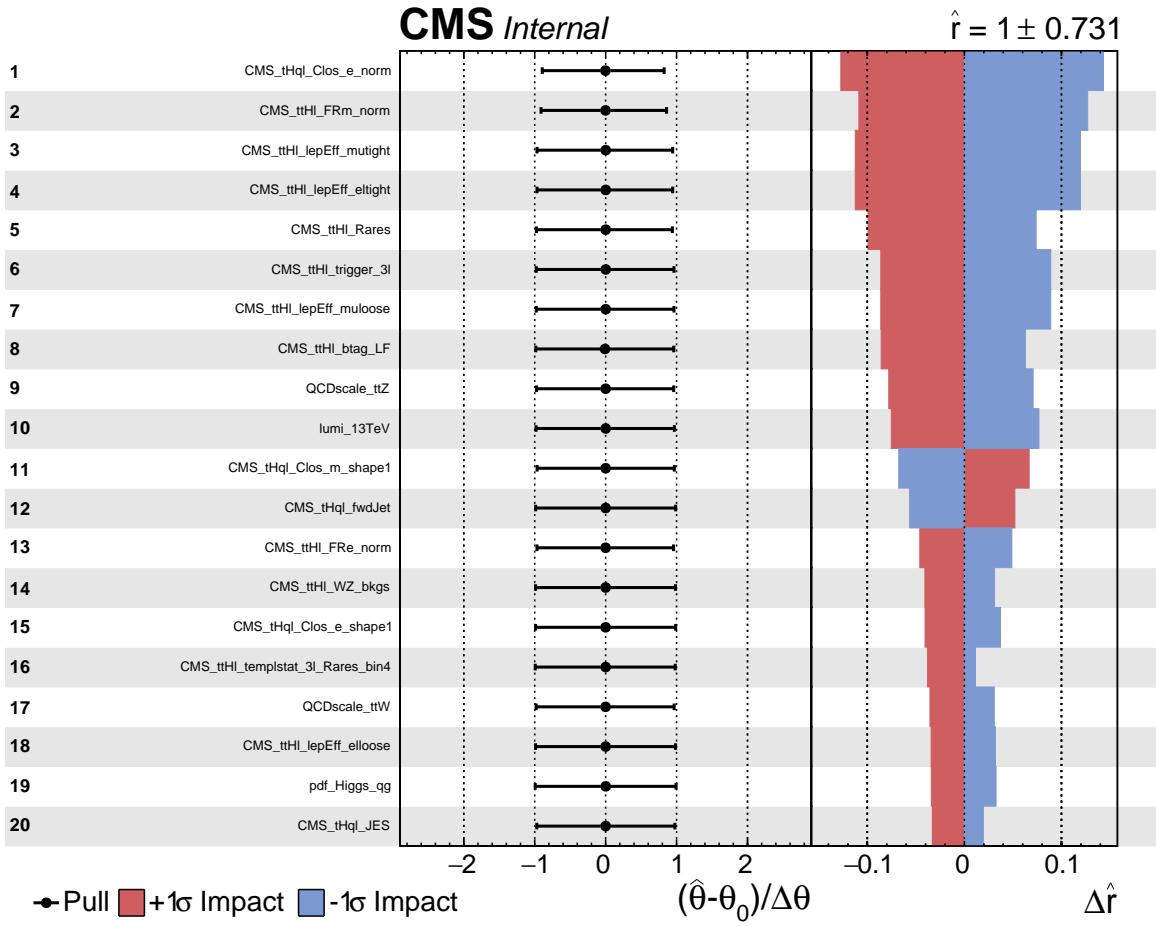
3611 The impact of the data/MC disagreement for forward jet  $\eta$  is observed to reduce with  
3612 higher  $p_T$  cuts; Figures F.1, F.2 and F.3 show this reduction in the impact of the  
3613 forward jet  $\eta$  nuisance in the fit.



**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>3614</sup> **Appendix G**

<sup>3615</sup> **Cross sections and Branching**

<sup>3616</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>0.1068</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>0.197</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>0.356</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>0.508</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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