

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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6 A DISSERTATION

7 Presented to the Faculty of
8 The Graduate College at the University of Nebraska
9 In Partial Fulfilment of Requirements
10 For the Degree of Doctor of Philosophy

11 Major: Physics and Astronomy

12 Under the Supervision of Kenneth Bloom and Aaron Dominguez

13 Lincoln, Nebraska

14 July, 2018

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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 ± 1.25 to ± 1.60 are excluded at 95% C.L., assuming $k_V = 1.0$.

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²⁹³ **Chapter 1**

²⁹⁴ **Theoretical approach**

²⁹⁵ **1.1 Introduction**

²⁹⁶ The physical description of the universe is a challenge that physicists have faced by
²⁹⁷ making theories that refine existing principles and proposing new ones in an attempt
²⁹⁸ to embrace emerging facts and phenomena.

²⁹⁹ At the end of 1940s Julian Schwinger [1] and Richard P. Feynman [2], based on
³⁰⁰ the work of Sin-Itiro Tomonaga [3], developed an electromagnetic theory consistent
³⁰¹ with special relativity and quantum mechanics that describes how matter and light
³⁰² interact; the so-called *quantum electrodynamics* (QED) was born.

³⁰³ QED has become the blueprint for developing theories that describe the universe.
³⁰⁴ It was the first example of a quantum field theory (QFT), which is the theoretical
³⁰⁵ framework for building quantum mechanical models that describes particles and their
³⁰⁶ interactions. QFT is composed of a set of mathematical tools that combines classical
³⁰⁷ fields, special relativity and quantum mechanics, while keeping the quantum point
³⁰⁸ particles and locality ideas.

³⁰⁹ This chapter gives an overview of the standard model of particle physics, starting

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

314 1.2 Standard model of particle physics

315 The *standard model of particle physics (SM)* describes particle physics at the funda-
 316 mental level in terms of a collection of interacting particles and fields. The full picture
 317 of the SM is composed of three fields¹ whose excitations are interpreted as particles
 318 called mediators or force-carriers, a set of fields whose excitations are interpreted as
 319 elementary particles interacting through the exchange of those mediators, and a field
 320 that gives the mass to elementary particles. Figure 1.1 shows a scheme of the SM
 321 particles’ organization. In addition, for each of the particles in the scheme there exists
 322 an antiparticle with the same mass and opposite quantum numbers. The existence of
 323 antiparticles is a prediction of the relativistic quantum mechanics from the solution
 324 of the Dirac equation for which a negative energy solution is also possible. In some
 325 cases a particle is its own anti-particle, like photon or Higgs boson.

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

¹ 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

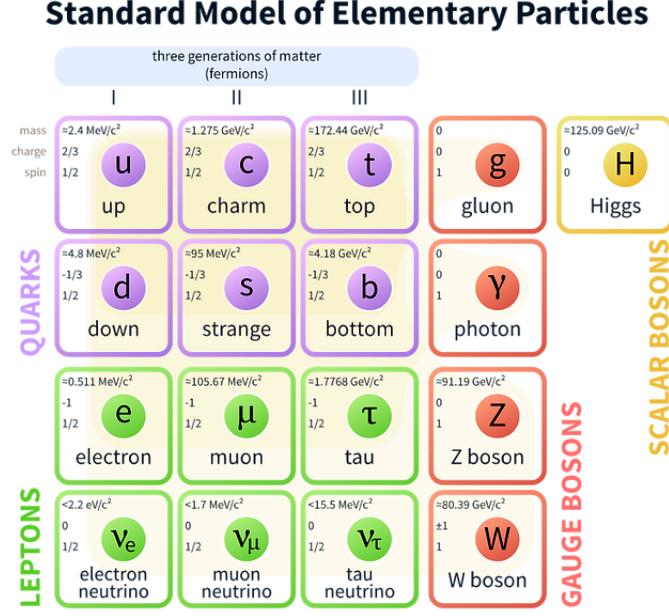


Figure 1.1: Schematic representation of the Standard Model of particle physics. The SM is a theoretical model intended to describe three of the four fundamental forces of the universe in terms of a set of particles and their interactions. [7].

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

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

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

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

345 **1.2.1 Fermions**

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

		Generation		
		1st	2nd	3rd
Leptons	Type	Charged	Electron (e)	Moun(μ)
	Neutral	Electron neutrino (ν_e)	Muon neutrino (ν_μ)	Tau neutrino (ν_τ)
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.

351

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

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

Lepton	Mass (MeV/c ²)	Quark	Mass (MeV/c ²)
e	0.51	u	2.2
μ	105.65	c	1.28×10^3
τ	1776.86	t	173.1×10^3
ν_e	Unknown	d	4.7
ν_μ	Unknown	s	96
τ_μ	Unknown	b	4.18×10^3

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.

361

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

364 1.2.1.1 Leptons

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

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

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

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

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

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

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

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

² 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.

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

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

Lepton	$Q(e)$	T_3	L_e	L_μ	L_τ	Lifetime (s)
Electron (e)	-1	-1/2	1	0	0	Stable
Electron neutrino(ν_e)	0	1/2	1	0	0	Unknown
Muon (μ)	-1	-1/2	0	1	0	2.19×10^{-6}
Muon neutrino (ν_μ)	0	1/2	0	1	0	Unknown
Tau (τ)	-1	-1/2	0	0	1	290.3×10^{-15}
Tau neutrino (ν_τ)	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.

409

410 1.2.1.2 Quarks

411 Quarks are the basic constituents of protons and neutrons. The way quarks join to
 412 form bound states, called *hadrons*, is through the SI. Quarks are affected by all the
 413 fundamental interactions which means that they carry all the four types of charges:
 414 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.

415

416 Table 1.4 summarizes the features of quarks, among which the most remarkable
 417 is their fractional electric charge. Note that fractional charge is not a problem, given
 418 that quarks are not found isolated, but serves to explain how composed particles are
 419 formed out of two or more valence quarks³.

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

- 426 • one quark with a color charge is attracted by an anti-quark with the correspond-
 427 ing anti-color charge forming a colorless particle called a *meson*.

 428 • three quarks (anti-quarks) with different color (anti-color) charges are attracted
 429 among them forming a colorless particle called a *baryon (anti-baryon)*.

³ 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.

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

436 In the first version of the quark model (1964), M. Gell-Mann [12] and G. Zweig
 437 [13, 14] developed a consistent way to classify hadrons according to their properties.
 438 Only three quarks (u, d, s) were involved in a scheme in which all baryons have baryon
 439 number $B=1$ and therefore quarks have $B=1/3$; non-baryons have $B=0$. Baryon
 440 number is conserved in SI and EI which means that single quarks cannot be created
 441 but in pairs $q - \bar{q}$.

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

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

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

446 There are six quark flavors organized in three generations (see Table 1.1) fol-
 447 lowing a mass hierarchy which, again, implies that higher generations decay to first
 448 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	$4/3$	ν_{eR}	$\nu_{\mu R}$	$\nu_{\tau R}$		
	d'_R	s'_R	b'_R	0	$-2/3$	e_R	μ_R	τ_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.

449

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

456

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

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

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

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

463 CKM matrix is a 3×3 unitary matrix parametrized by three mixing angles and
 464 the *CP-mixing phase*; the latter is the parameter responsible for the Charge-Parity

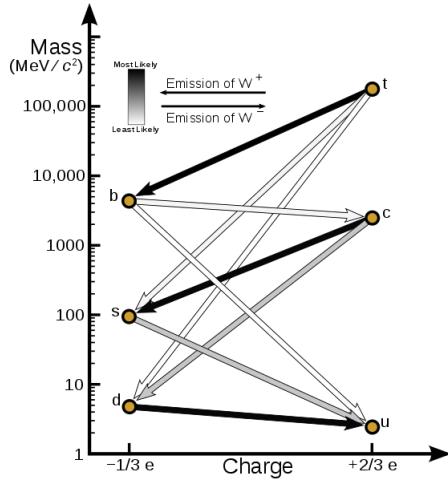


Figure 1.2: Transformations between quarks through the exchange of a WI. Higher generations quarks decay to first generation quarks by emitting a W boson. The arrow color indicates the likelihood of the transition according to the grey scale in the top left side which represent the CKM matrix parameters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

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

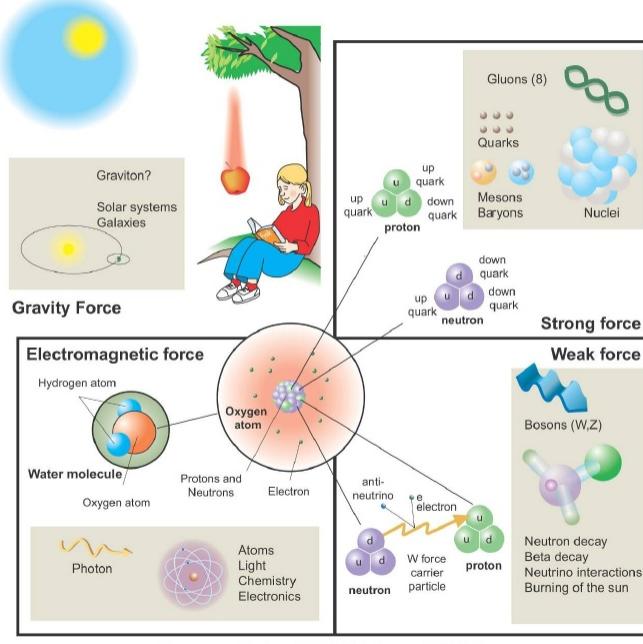
469 1.2.2 Fundamental interactions

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

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

Fundamental interactions.

Illustration: Typoform



Summer School KPI 15 August 2009

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.

477 posed of two or more valence quarks⁴. Quarks have fractional electric charge
 478 which means that they are subject to electromagnetic interaction and in the case
 479 of the proton they should break apart due to electrostatic repulsion; however,
 480 quarks are held together inside the hadrons against their electrostatic repulsion
 481 by the *Strong Force* through the exchange of *gluons*. The analog to the electric
 482 charge is the *color charge*. Electrons and photons are elementary particles as
 483 quarks but they don't carry color charge, therefore they are not subject to SI. A
 484 Feynman diagram for gluon exchange between quarks is shown in Figure 1.4b.

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

⁴ Particles made of four and five quarks are exotic states not so common.

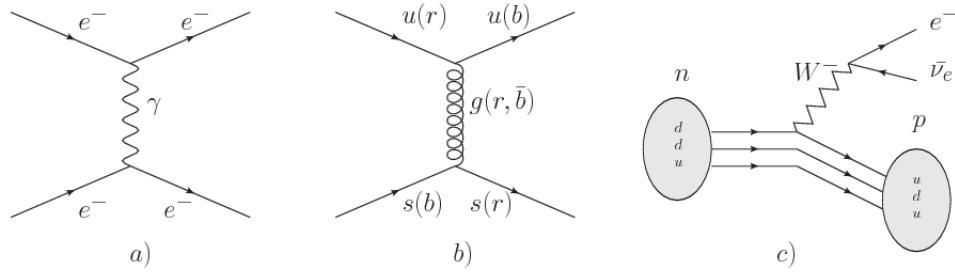


Figure 1.4: Feynman diagrams representing the interactions in SM; a) EI: e - e scattering; b) SI: gluon exchange between quarks ; c) WI: β -decay

487 within the sun. Quarks and leptons are the particles affected by the weak
 488 interaction; they possess a property called *flavor charge* (see 1.2.1) which can
 489 be changed by emitting or absorbing one weak force mediator. There are three
 490 mediators of the *weak force* known as Z boson in the case of electrically neutral
 491 flavor changes and W^\pm bosons in the case of electrically charged flavor changes.
 492 The *weak isospin* is the WI analog to electric charge in EI, and color charge in
 493 SI, and defines how quarks and leptons are affected by the weak force. Figure
 494 1.4c. shows the Feynman diagram of β -decay where a neutron (n) is transformed
 495 in a proton (p) by emitting a W^- particle.

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

505 force⁵.

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].

506

507 Table 1.6 summarizes the main features of the fundamental interactions. The
 508 strength of the interactions is represented by the coupling constants which depend
 509 on the energy scale at which the interaction is evaluated, therefore, it is the relative
 510 strength of the fundamental forces that reveals the meaning of strong and weak; in
 511 a context where the relative strength of the SI is 1, the EI is about hundred times
 512 weaker and WI is about million times weaker than the SI. A good description on how
 513 the relative strength and range of the fundamental interactions are calculated can
 514 be found in References [20, 21]. In the everyday life, only EI and GI are explicitly
 515 experienced due to the range of these interactions; i.e., at the human scale distances
 516 only EI and GI have appreciable effects, in contrast to SI which at distances greater
 517 than 10^{-15} m become negligible. Is it important to clarify that the weakness of the
 518 WI is attributed to the fact that its mediators are highly massive which affects the
 519 propagators of the interaction, as a result, the effect of the coupling constant is
 520 reduced.

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

521 **1.2.3 Gauge invariance.**

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

- 525 • Lorentz invariance: independence on the reference frame.
- 526 • Locality: interacting fields are evaluated at the same space-time point to avoid
 527 action at a distance.
- 528 • Renormalizability: physical predictions are finite and well defined.
- 529 • Particle spectrum, symmetries and conservation laws already known must emerge
 530 from the theory.
- 531 • Local gauge invariance.

532 The gauge invariance requirement reflects the fact that the fundamental fields
 533 cannot be directly measured but associated fields which are the observables. Electric
 534 (**E**) and magnetic (**B**) fields in CED are associated with the electric scalar potential
 535 V and the vector potential **A**. In particular, **E** can be obtained by measuring the
 536 change in the space of the scalar potential (ΔV); however, two scalar potentials
 537 differing by a constant f correspond to the same electric field. The same happens
 538 in the case of the vector potential **A**; thus, different configurations of the associated
 539 fields result in the same set of values of the observables. The freedom in choosing one
 540 particular configuration is known as *gauge freedom*; the transformation law connecting
 541 two configurations is known as *gauge transformation* and the fact that the observables
 542 are not affected by a gauge transformation is called *gauge invariance*.

543 When the gauge transformation:

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

544 is applied to Maxwell equations, they are still satisfied and the fields remain invariant.
 545 Thus, CED is invariant under gauge transformations and is called a *gauge theory*.
 546 The set of all gauge transformations form the *symmetry group* of the theory, which
 547 according to the group theory, has a set of *group generators*. The number of group
 548 generators determine the number of *gauge fields* of the theory.

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

556 As will be detailed in Section 1.3, interactions between particles in a system can
 557 be obtained by considering first the Lagrangian density of free particles in the sys-
 558 tem, which of course is incomplete because the interaction terms have been left out,
 559 and demanding global phase transformation invariance. Global phase transforma-
 560 tion invariance means that a gauge transformation is performed identically to every point
 561 in the space⁶ and the Lagrangian remains invariant. Then, the global transforma-
 562 tion is promoted to a local phase transformation (this time the gauge transformation
 563 depends on the position in space) and again invariance is required.

⁶ Here space corresponds to the 4-dimensional space i.e. space-time.

564 Due to the space dependence of the local transformation, the Lagrangian density is
 565 not invariant anymore. In order to reinstate the gauge invariance, the gauge covariant
 566 derivative is introduced in the Lagrangian and with it the gauge field responsible for
 567 the interaction between particles in the system. The new Lagrangian density is gauge
 568 invariant, includes the interaction terms needed to account for the interactions and
 569 provides a way to explain the interaction between particles through the exchange of
 570 the gauge boson.

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

573 1.2.4 Gauge bosons

574 The importance of the gauge bosons comes from the fact that they are the force
 575 mediators or force carriers. The features of the gauge bosons reflect those of the fields
 576 they represent and they are extracted from the Lagrangian density used to describe
 577 the interactions. In Section 1.3, it will be shown how the gauge bosons of the EI and
 578 WI emerge from the electroweak Lagrangian. The SI gauge bosons features are also
 579 extracted from the SI Lagrangian but it is not detailed in this document. The main
 580 features of the SM gauge bosons will be briefly presented below and summarized in
 581 Table 1.7.

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

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

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

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

602

603 1.3 Electroweak unification and the Higgs 604 mechanism

605 Physicists dream of building a theory that contains all the interactions in one single
 606 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.

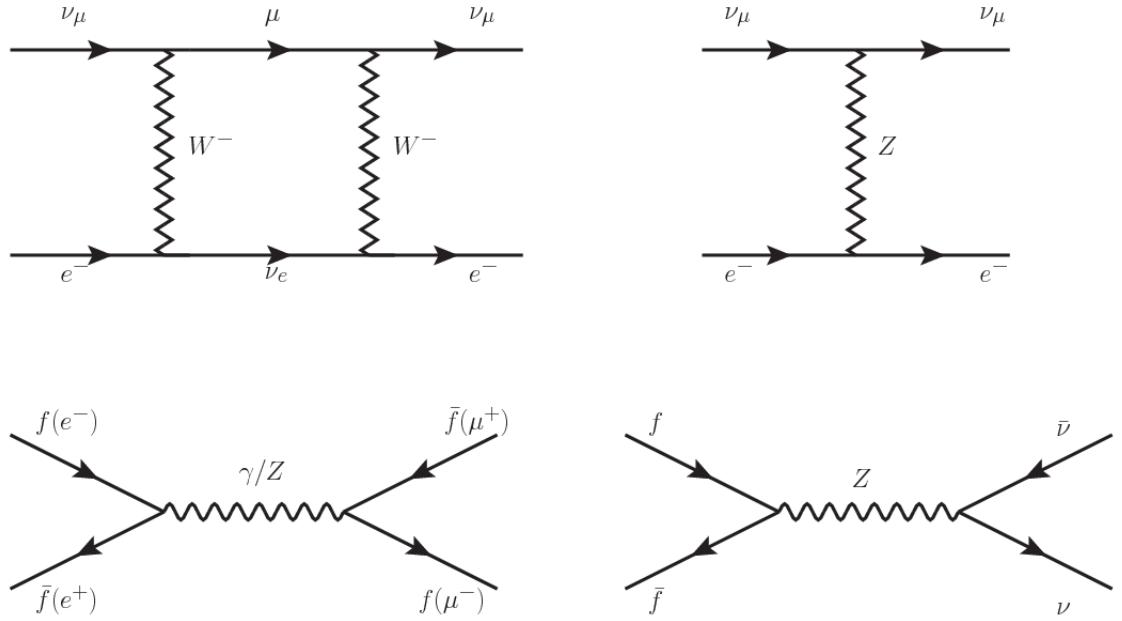


Figure 1.5: Top: $\nu_\mu - e^-$ scattering going through charged currents (left) and neutral currents (right). Bottom: neutral current processes for charged fermions (left) and involving neutrinos (right). While neutral current processes involving only charged fermions can proceed through EI or WI,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

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

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

630 The prescription to build a gauge theory of the WI consists of proposing a free
 631 field Lagrangian density that includes the particles involved; next, by requesting
 632 invariance under global phase transformations first and generalizing to local phase
 633 transformations invariance later, the conserved currents are identified and interactions
 634 are generated by introducing gauge fields. Given that the goal is to include the EI
 635 and WI in a single theory, the group symmetry considered should be a combination of
 636 $SU(2)_L$ and $U(1)_{em}$, however the latter cannot be used directly because the EI treats
 637 left and right-handed particles indistinctly in contrast to the former. Fortunately, the
 638 weak hypercharge, which is a combination of the weak isospin and the electric charge
 639 (Eqn. 1.2) is suitable to be used since it is conserved by the EI and WI. Thus, the
 640 symmetry group to be considered is

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

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

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

643 Given the first generation of leptons

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

644 the charged fermionic currents are given by

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

645 and the free Lagrangian is given by

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

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

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

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

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

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

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

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

659 with σ_i the Pauli matrices and y_i the weak hypercharges. In order to promote the
 660 transformations from global to local while keeping the invariance, it is required that
 661 $\alpha^i = \alpha^i(x)$, $\beta = \beta(x)$ and the replacement of the ordinary derivatives by the covariant
 662 derivatives

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

677 In order to evaluate the electroweak interactions modeled by an isos triplet field
 678 W_μ^i that couples to isospin currents J_μ^i with strength g and additionally the singlet
 679 field B_μ which couples to the weak hypercharge current J_μ^Y with strength $g'/2$. The
 680 interaction Lagrangian density to be considered is

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

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

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

684 The same happens with the gauge fields W_μ^i which are related to the mass eigen-
 685 states W^\pm by

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

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

691 current (j_μ^{em}), indicating that there is a relation between them and resembling the
 692 Gell-Mann-Nishijima formula 1.2 adapted to electroweak interactions

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

693 Just as Q generates the $U(1)_{em}$ symmetry, the weak hypercharge generates the
 694 $U(1)_Y$ symmetry as said before. It is possible to write the relationship in terms of
 695 the currents as

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

696 The neutral gauge fields W_μ^3 and B_μ cannot be directly identified with the Z
 697 and the photon fields since the photon interacts similarly with left and right-handed
 698 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 θ_W is known as the *Weinberg angle*. The interaction Lagrangian is now given by

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

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

700 electromagnetic interaction under the condition

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

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

702

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

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

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

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

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

711 1.3.1 Spontaneous symmetry breaking (SSB)

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

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

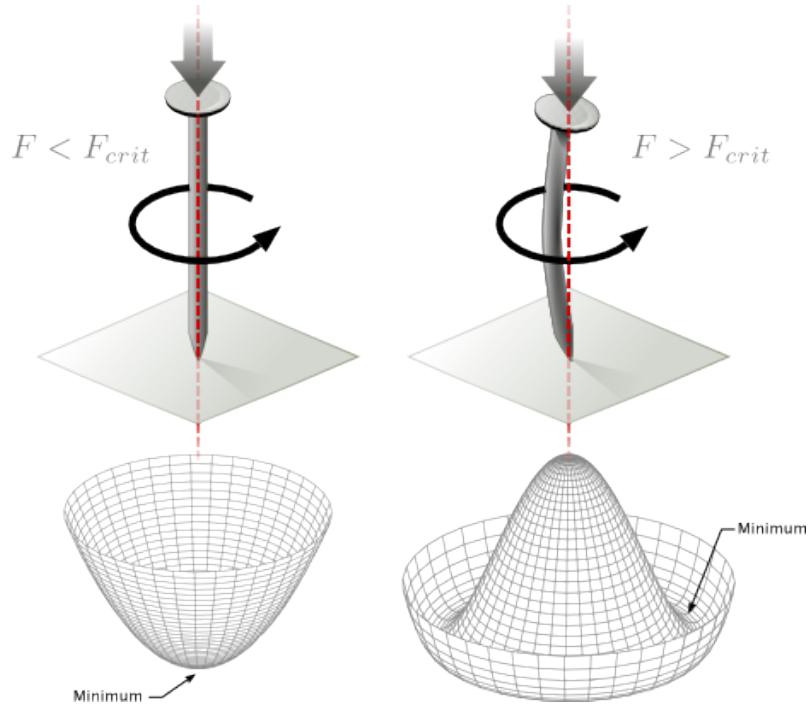


Figure 1.6: Spontaneous symmetry breaking mechanism. The steel nail, subject to an external force (top left), has rotational symmetry with respect to its axis. When the external force overcomes a critical value the nail buckles (top right) choosing a minimal energy state (ground state) and thus *breaking 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].

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

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

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

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

If $\mu^2 > 0$ the potential has only one minimum at $\phi = 0$ and describes a scalar field with mass μ . 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.

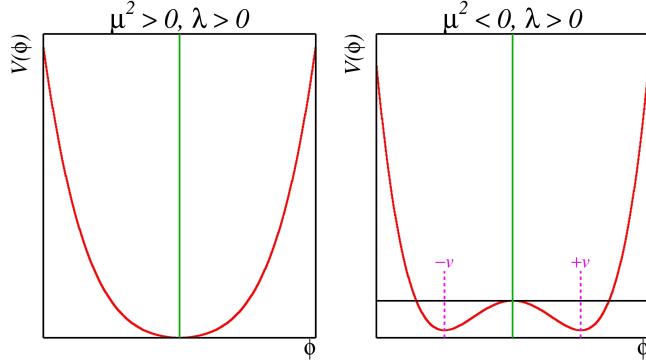


Figure 1.7: Shape of the potential $V(\phi)$ for $\lambda > 0$ and: $\mu^2 > 0$ (left) and $\mu^2 < 0$ (right). The case $\mu^2 < 0$ corresponds to the potential suitable for introducing the SSB mechanism by choosing one of the two ground states which are connected via reflection symmetry. [31].

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 ξ -direction which makes possible the occurrence of the SSB by choosing an arbitrary ground state; for instance, $\xi = 0$, i.e. $\phi_1 = v, \phi_2 = 0$

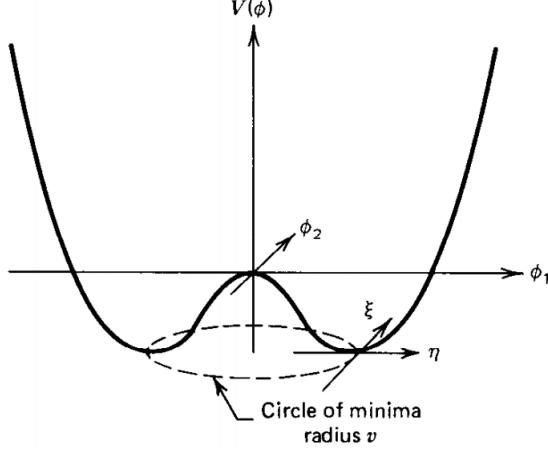


Figure 1.8: Potential for complex scalar field. There is a circle of minima of radius v along the ξ -direction [6].

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

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

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

737 which when substituted into Eqn. 1.33 produces a Lagrangian in terms of the new
 738 fields η and ξ

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

739 where the last two terms represent the interactions and self-interaction between the
 740 two fields η and ξ . The particular feature of the SSB mechanism is revealed when
 741 looking to the first three terms of \mathcal{L}' . Before the SSB, only the massless ϕ field is

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

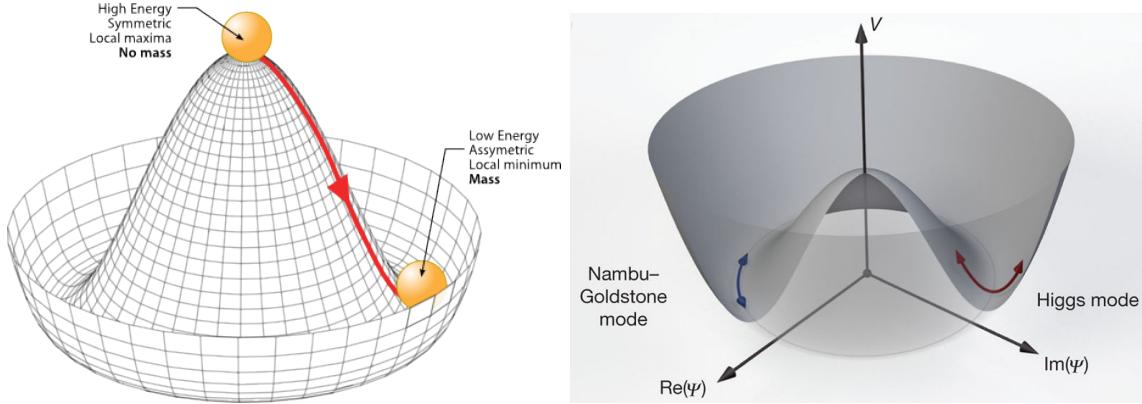


Figure 1.9: SSB mechanism for a complex scalar field [31, 32].

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

754 1.3.2 Higgs mechanism

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

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

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

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

760 ϕ has to be an isospin doublet of complex scalar fields so it preserves the G invariance;
 761 thus ϕ can be defined as:

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

762 The minima of the potential are defined by

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

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

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

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

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

771 The next step is to expand ϕ about the chosen ground state as:

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

772 to describe fluctuations from the ground state ϕ_0 . The fields $\theta_i(x)$ represent the
 773 Nambu-Goldstone bosons while $H(x)$ is known as *Higgs field*. The fundamental fea-
 774 ture of the parametrization used is that the dependence on the $\theta_i(x)$ fields is factored
 775 out in a global phase that can be eliminated by taking the physical *unitary gauge*
 776 $\theta_i(x) = 0$. Therefore the expansion about the ground state is given by:

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

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

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

791 **1.3.3 Masses of the gauge bosons**

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

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

794 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_μ and A_μ in order to be compared to the typical mass terms for neutral bosons, therefore using Eqn. 1.29

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

795 and then

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

796 **1.3.4 Masses of the fermions**

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

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

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

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

801

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

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

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

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

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

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

810 of \mathcal{L}_{Yq} is:

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

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

813 1.3.5 The Higgs field

814 After the characterization of the fermions and gauge bosons as well as their interac-
815 tions, it is necessary to characterize the Higgs field itself. The Lagrangian \mathcal{L}_S in Eqn.
816 1.37 written in terms of the gauge bosons is given by

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

817

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

818

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

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

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

821 however, it is not predicted by the theory either. The experimental measurement of
822 the Higgs boson mass have been performed by the *Compact Muon Solenoid (CMS)*
823 experiment and the *A Toroidal LHC Appartus (ATLAS)* experiments at the *Large
824 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^2)	$125.09 \pm 0.21 \text{ (stat.)} \pm 0.11 \text{ (syst.)}$

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

1.3.6 Production of Higgs bosons at LHC

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

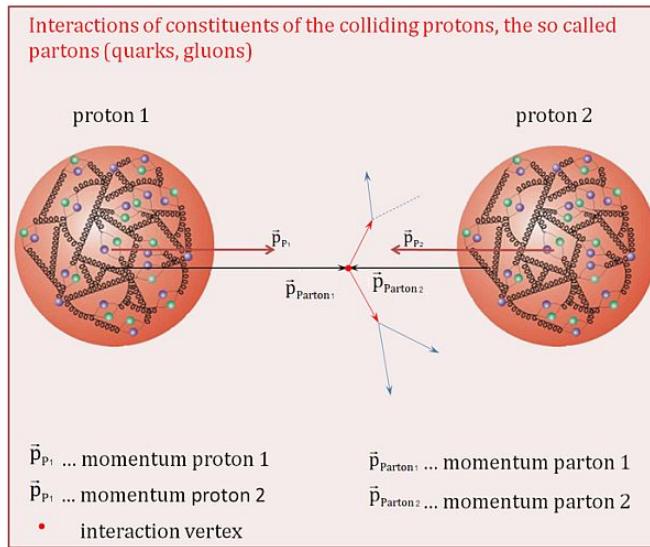


Figure 1.10: Proton-proton collision. Protons are composed of 3 valence quarks, a sea of quarks and gluons; therefore in a proton-proton collision, quarks and gluons are those who collide. [39].

829

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

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

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

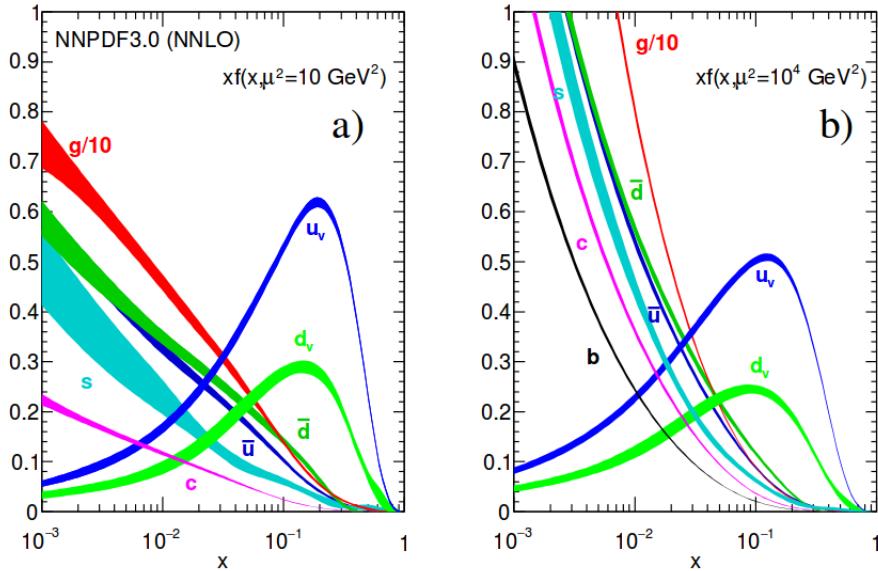


Figure 1.11: Proton PDFs for two values of Q^2 : left. $\mu^2 = Q^2 = 10 \text{ GeV}^2$, right. $\mu^2 = Q^2 = 10^4 \text{ GeV}^2$. u_v and d_v correspond to the u and d valence quarks, $s, c, b, \bar{u}, \bar{d}$ correspond to sea quarks, and g corresponds to gluons. Note that gluons carry a high fraction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

845 In physics, a common approach to study complex systems consists of starting
 846 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.

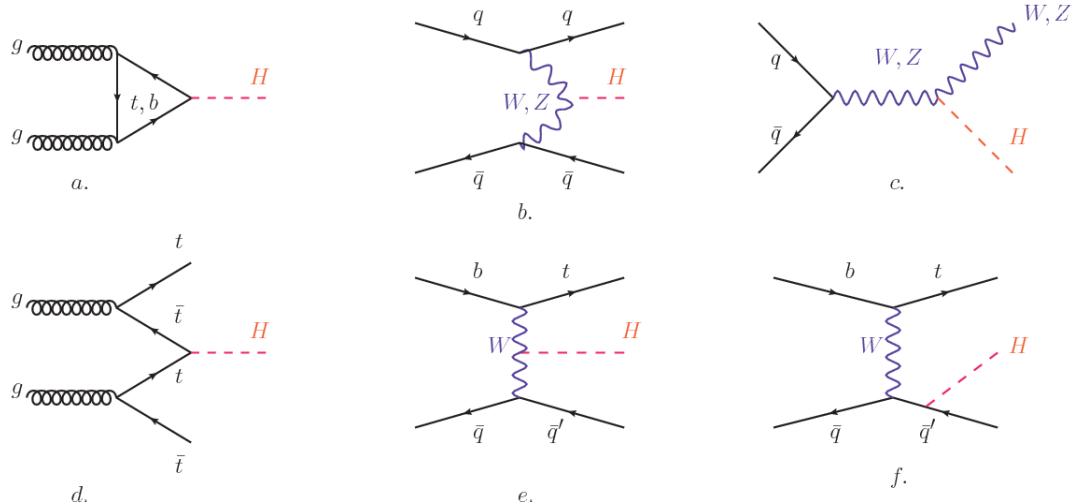


Figure 1.12: Main Higgs boson production mechanism Feynman diagrams. a. gluon-gluon fusion, b. vector boson fusion (VBF), c. Higgs-strahlung, d. Associated production with a top or bottom quark pair, e-f. associated production with a single top quark.

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.

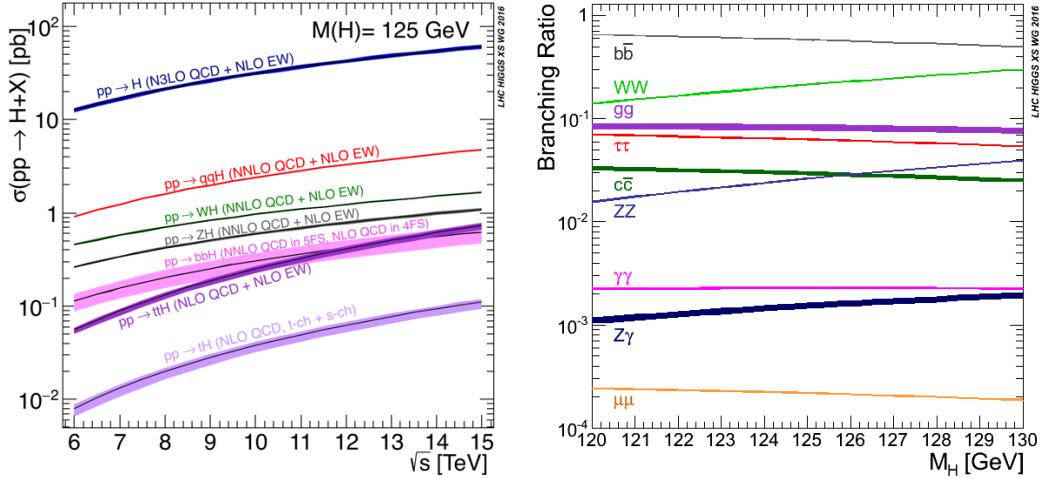


Figure 1.13: Higgs boson production cross sections (left) and decay branching ratios (right) for the main mechanisms. The VBF is indicated as qqH [40].

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

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

880 Vector boson fusion (Figure 1.12b and $pp \rightarrow qqH$ in Figure 1.13) has the second
 881 largest production cross section. The scattering of two fermions is mediated by a weak
 882 gauge boson which later emits a Higgs boson. In the final state, the two fermions tend
 883 to be located in the central region of the detector; this kind of features are generally
 884 used as a signature when analyzing the datasets provided by the experiments⁷.

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

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

894 1.3.7 Higgs boson decay channels

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

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

901 is presented; the largest predicted BR corresponds to the $b\bar{b}$ pair decay channel (see
 902 Table 1.9) given that it is the heaviest particle pair whose on-shell⁸ production is
 903 kinematically allowed in the decay.

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

904

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

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

⁸ 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.

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

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

921 **1.4 Experimental status of the anomalous
 922 Higgs-fermion coupling**

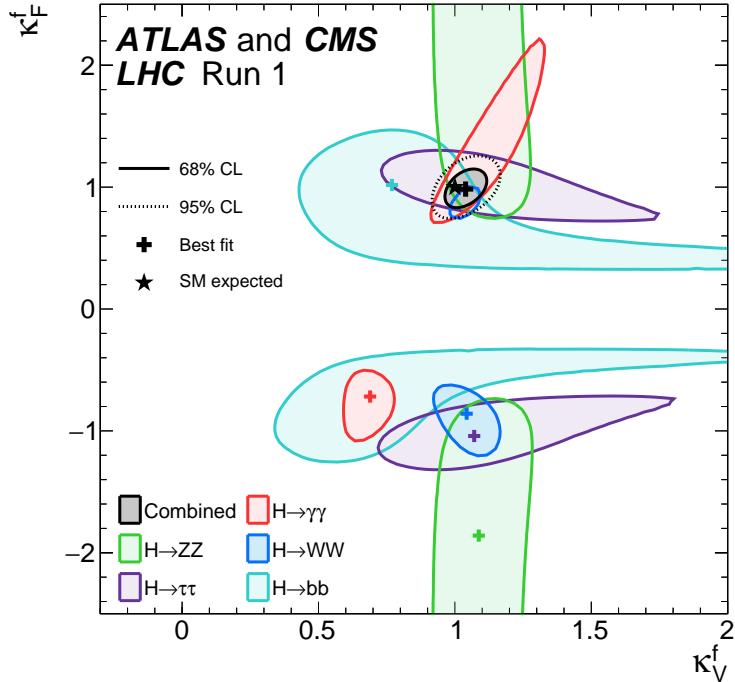


Figure 1.14: Combination of the ATLAS and CMS fits for coupling modifiers $\kappa_t - \kappa_V$; also shown the individual decay channels combination and their global combination. No assumptions have been made on the sign of the coupling modifiers [44].

923 ATLAS and CMS have performed analyses of the anomalous Higgs-fermion cou-
 924 pling by making likelihood scans for the two coupling modifiers, κ_f and κ_V , under
 925 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
 926 result of the combination of ATLAS and CMS fits; also the individual decay channels
 927 combination and the global combination results are shown. Note that from this plot
 928 there is limited information on the sign of the coupling since the only information
 929 available about the sign of the coupling comes from decays rather than production.

930 While all the channels are compatible for positive values of the modifiers, for
 931 negative values of κ_f there is no compatibility. The best fit for individual channels
 932 is compatible with negative values of κ_f except for the $H \rightarrow bb$ channel. The best
 933 fit for the combination yields $\kappa_f \geq 0$, in contrast to the yields from the individual
 934 channels; the reason of this yield resides in the $H \rightarrow \gamma\gamma$ coupling. $H \rightarrow \gamma\gamma$ decay
 935 proceeds through a loop of either top quarks or W bosons, hence, this channel is
 936 sensitive to κ_t thanks to the interference of these two amplitude contributions; under
 937 the assumption that no beyond SM particles take part in the loops, a flipped sign
 938 of κ_t will increase the $H \rightarrow \gamma\gamma$ branching fraction by a factor of ~ 2.4 which is not
 939 supported by measurements; thus, this large asymmetry between the positive and
 940 negative coupling ratios in the $H \rightarrow \gamma\gamma$ channel drives the yield of the global fit and
 941 would mean that the anomalous H-t coupling is excluded as stated in Reference [44],
 942 but there is a caveat, this exclusion holds only if no new particles contribute to the
 943 loop in the main diagram for that decay.

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

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

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

956 1.5 Associated production of a Higgs boson and a 957 single top quark

958 The production of Higgs boson in association with a top quark has been extensively
 959 studied [47, 49–52]. While measurements of the main Higgs production mechanisms
 960 rates are sensitive to the strength of the Higgs coupling to W boson or top quark,
 961 they are not sensitive to the relative sign between the two couplings. In this thesis,
 962 the Higgs boson production mechanism explored is the associated production with a
 963 single top quark (tH) which offers sensitivity to the relative sign of the Higgs couplings
 964 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

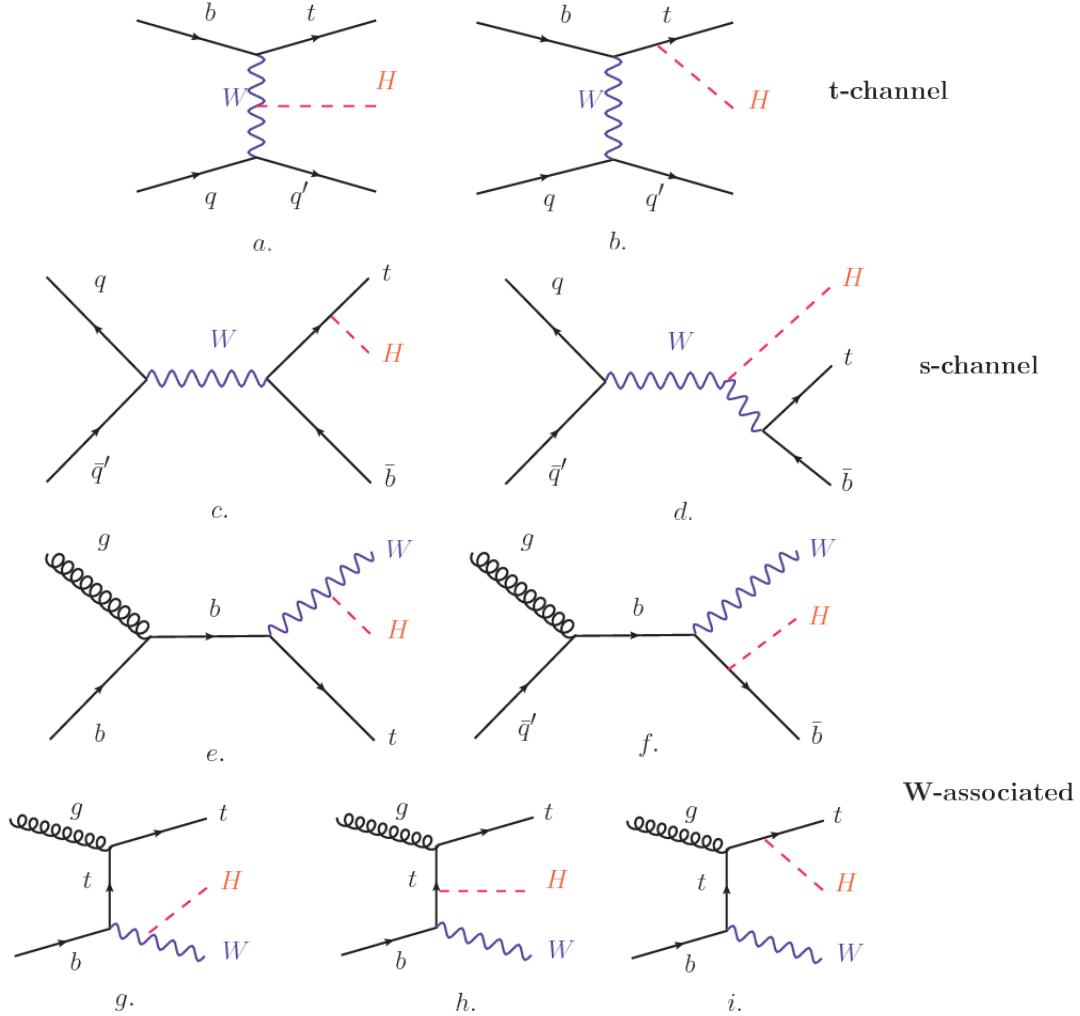


Figure 1.15: Associated Higgs boson production with a top quark mechanism Feynman diagrams. a.,b. t-channel (tHq), c.,d. s-channel (tHb), e-i. W-associated.

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

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

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

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

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

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

970 The tH production, where Higgs boson can be radiated either from the top quark or
 971 from the W boson, is represented by the leading order Feynman diagrams in Figure
 972 1.15. The cross section for the tH process is calculated, as usual, summing over
 973 the contributions from the different Feynman diagrams; therefore it depends on the
 974 interference between the contributions. In the SM, the interference for t-channel (tHq
 975 process) and W-associated (tHW process) production is destructive [49] resulting in
 976 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].

977

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

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

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

987 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
 988 possible deviations of the couplings from the SM values, Higgs-Vector boson (H-
 989 W) and Higgs-top (H-t) respectively, from the SM couplings; $s = (p_W + p_b)^2$, $t =$
 990 $(p_W - p_H)^2$, φ is the Higgs azimuthal angle around the z axis taken parallel to the
 991 direction of motion of the incoming W; A and B are functions describing the weak
 992 interaction in terms of the chiral states (ξ_t, ξ_b) of the quarks b and t . Terms that
 993 vanish in the high energy limit have been neglected as well as the Higgs and b quark
 994 masses⁹.

995 The scattering amplitude grows with energy like \sqrt{s} for $\kappa_V \neq \kappa_t$, in contrast to
 996 the SM ($\kappa_t = \kappa_V = 1$), where the first term in 1.62 cancels out and the amplitude
 997 is constant for large s ; therefore, a deviation from the SM predictions represents an
 998 enhancement in the tHq cross section. In particular, for a SM H-W coupling and a
 999 H-t coupling of inverted sign with respect to the SM ($\kappa_V = -\kappa_t = 1$) the tHq cross
 1000 section is enhanced by a factor greater 10 as seen in the Figure 1.16 taken from
 1001 Reference [51]; Reference [56] has reported similar enhancement results.

1002 A similar analysis is valid for the W-associated channel but, in that case, the in-
 1003 terference is more complicated since there are more than two contributions and an ad-
 1004 ditional interference with the production of Higgs boson and a top pair process($t\bar{t}H$).
 1005 The calculations are made using the so-called Diagram Removal (DR) technique where

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

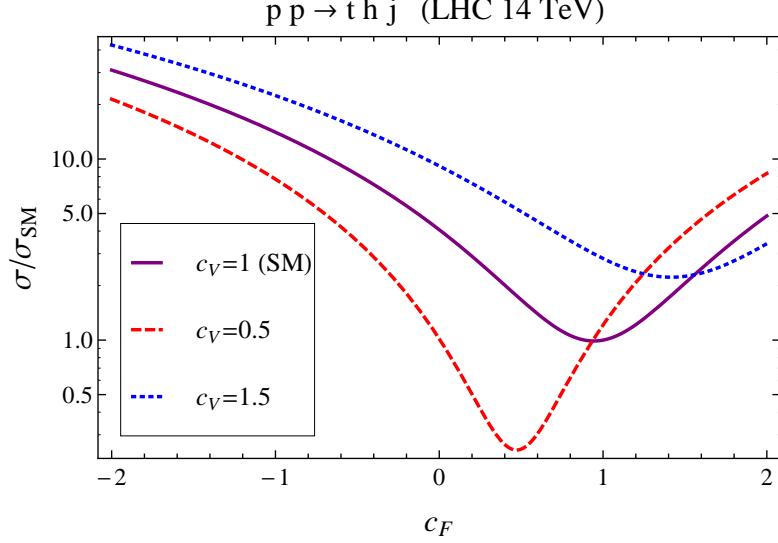


Figure 1.16: Cross section for tHq process as a function of κ_t , normalized to the SM, for three values of κ_V . In the plot c_f refers to the Higgs-fermion coupling which is dominated by the H-t coupling and represented here by κ_t . Solid, dashed and dotted lines correspond to $c_V \rightarrow \kappa_V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

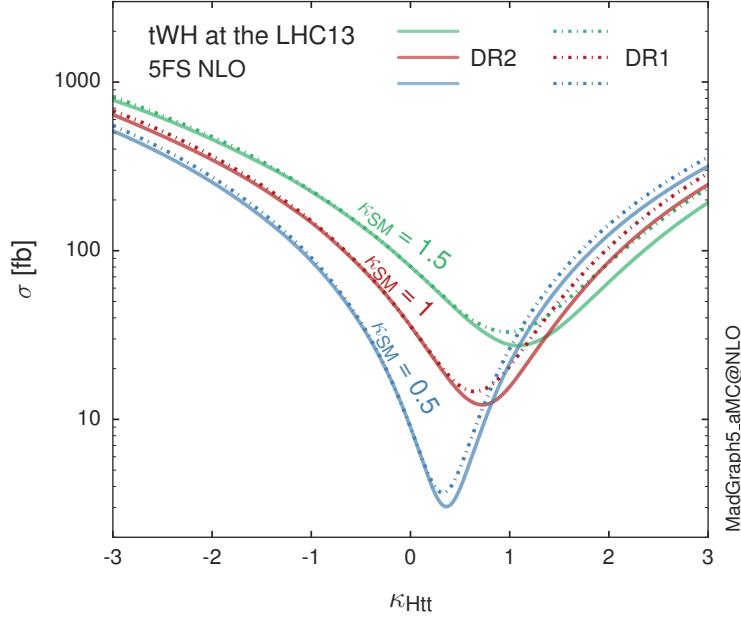


Figure 1.17: Cross section for tHW process as a function of κ_{Htt} , for three values of κ_{SM} at $\sqrt{s} = 13$ TeV. $\kappa_{Htt}^2 = \sigma_{Htt}/\sigma_{Htt}^{SM}$ is a simple re-scaling of the SM Higgs interactions.

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	≈ 17.4	≈ 252.7
	14	≈ 80.4	≈ 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	≈ 71.8	≈ 893
$\sigma^{LO}(tHW)(fb)$ [56]	14	≈ 16.0	≈ 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	$21.72^{+6.52\%}_{-5.24\%}$	≈ 150
$\sigma^{NLO}DR2(tHW)(fb)$ [48]	13	$16.28^{+7.34\%}_{-15.13\%}$	≈ 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.

1014

1015 1.6 CP-mixing in tH processes

1016 In addition to the sensitivity to sign of the H-t coupling, the tHq and tHW processes
 1017 have been proposed as a tool to investigate the possibility of a H-t coupling that does

1018 not conserve CP [47, 48, 58].

1019 In this thesis, the sensitivity of tH processes to CP-mixing is also studied on the
 1020 basis of References [47, 48] using the effective field theory framework where a generic
 1021 particle (X_0) of spin-0 and a general CP violating interaction with the top quark
 1022 (Htt coupling), can couple to scalar and pseudo-scalar fermionic densities. The H-W
 1023 interaction is assumed to be SM-like. The Lagrangian modeling the H-t interaction
 1024 is given by

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

1025 where α is the CP-mixing phase, $c_\alpha \equiv \cos \alpha$ and $s_\alpha \equiv \sin \alpha$, κ_{Htt} and κ_{Att} are real
 1026 dimensionless re-scaling parameters¹⁰ used to parametrize the magnitude of the CP-
 1027 violating and CP-conserving parts of the amplitude. The model defines $g_{Htt} =$
 1028 $g_{Att} = m_t/v = y_t/\sqrt{2}$ with $v \sim 246$ GeV the Higgs vacuum expectation value. In
 1029 this parametrization, three special cases can be recovered

1030 • CP-even coupling $\rightarrow \alpha = 0^\circ$

1031 • CP-odd coupling $\rightarrow \alpha = 90^\circ$

1032 • SM coupling $\rightarrow \alpha = 0^\circ$ and $\kappa_{Htt} = 1$

1033 The loop induced X_0 coupling to gluons can also be described in terms of the
 1034 parametrization above, according to

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

1035 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.

1036 Under the assumption that the top quark dominates the gluon-fusion process at LHC

¹⁰ analog to κ_t and κ_V

1037 energies, $\kappa_{Hgg} \rightarrow \kappa_{Htt}$ and $\kappa_{Agg} \rightarrow \kappa_{Att}$, so that the ratio between the gluon-gluon
 1038 fusion cross section for X_0 and for the SM Higgs prediction can be written as

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

1039 If the re-scaling parameters are set to

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

1040 the gluon-fusion SM cross section is reproduced for every value of the CP-mixing
 1041 angle α ; therefore, by imposing that condition to the Lagrangian density 1.63, the
 1042 CP-mixing angle is not constrained by current data. Figure 1.18 shows the NLO cross
 1043 sections for t-channel tX_0 (blue) and $t\bar{t}X_0$ (red) associated production processes as a
 1044 function of the CP-mixing angle α . X_0 is a generic spin-0 particle with top quark
 1045 CP-violating coupling. Re-scaling factors κ_{Htt} and κ_{Att} have been set to reproduce
 1046 the SM gluon-fusion cross sections.

1047 It is interesting to notice that the tX_0 cross section is enhanced, by a factor of
 1048 about 10, when a continuous rotation in the scalar-pseudoscalar plane is applied; this
 1049 enhancement is similar to the enhancement produced when the H-t coupling is flipped
 1050 in sign with respect to the SM ($y_t = -y_{t,SM}$ in the plot), as showed in Section 1.5. In
 1051 contrast, the degeneracy in the $t\bar{t}X_0$ cross section is still present given that it depends
 1052 quadratically on the H-t coupling, but more interesting is to notice that $t\bar{t}X_0$ cross
 1053 section is exceeded by tX_0 cross section after $\alpha \sim 60^\circ$.

1054 A similar parametrization can be used to investigate the tHW process sensitivity
 1055 to CP-violating H-t coupling. As said in 1.5, the interference in the W-associated
 1056 channel is more complicated because there are more than two contributions and also
 1057 there is interference with the $t\bar{t}H$ production process.

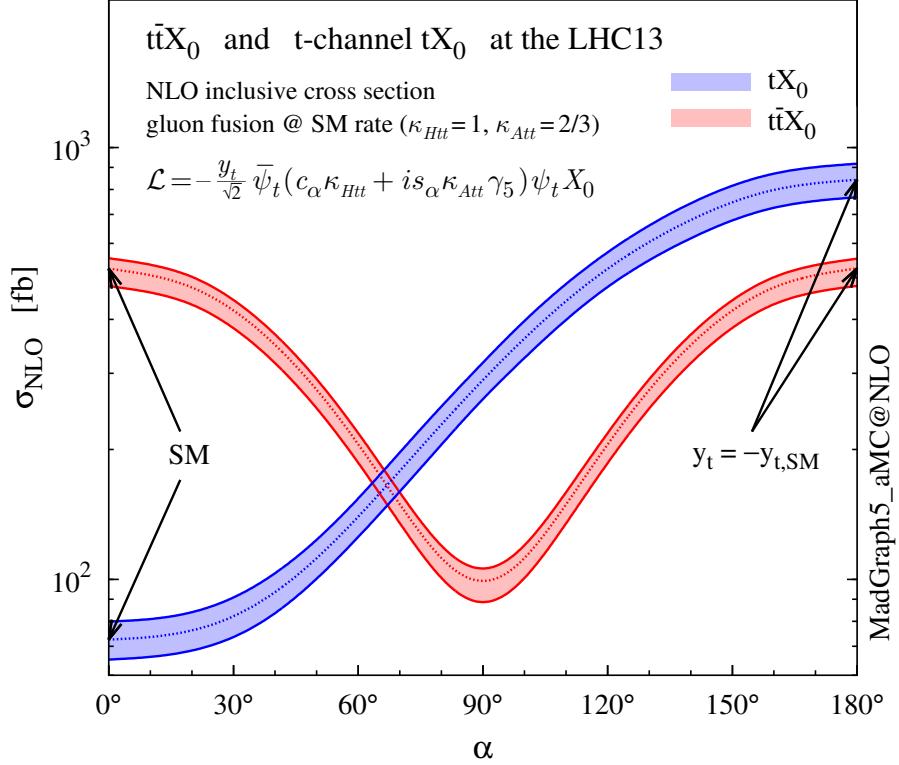


Figure 1.18: NLO cross sections for t-channel tX_0 (blue) and $t\bar{t}X_0$ (red) associated production processes as a function of the CP-mixing angle α . X_0 is a generic spin-0 particle with top quark CP-violating coupling [47].

1058 Figure 1.19 shows the NLO cross sections for t-channel tX_0 (blue), $t\bar{t}X_0$ (red)
 1059 associated production and for the combined $tWX_0 + t\bar{t}X_0 + \text{interference}$ (orange) as
 1060 a function of the CP-mixing angle. It is clear that the effect of the interference in the
 1061 combined case is the lifting of the degeneracy present in the $t\bar{t}X_0$ production. The
 1062 constructive interference enhances the cross section from about 500 fb at SM ($\alpha = 0$)
 1063 to about 600 fb ($\alpha = 180^\circ \rightarrow y_t = -y_{t,SM}$).

1064 An analysis combining tHq and tHW processes will be made in this thesis taking
 1065 advantage of the sensitivity improvement.

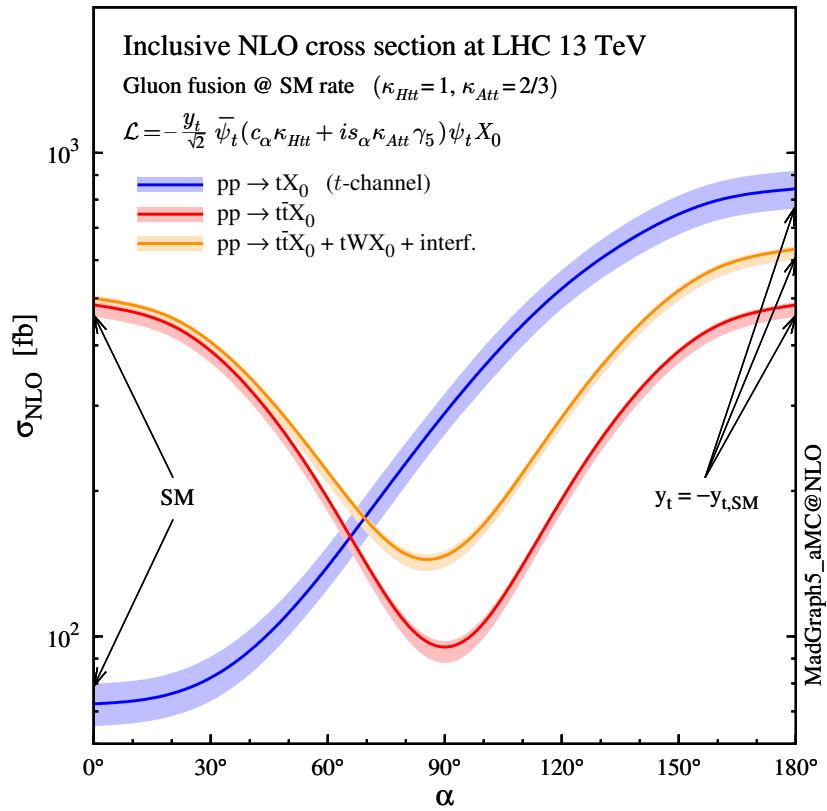


Figure 1.19: NLO cross sections for t-channel tX_0 (blue), $t\bar{t}X_0$ (red) associated production processes and combined $tWX_0 + t\bar{t}X_0$ (including interference) production as a function of the CP-mixing angle α [47].

1066 **Chapter 2**

1067 **The CMS experiment at the LHC**

1068 **2.1 Introduction**

1069 Located on the Swiss-French border, the European Council for Nuclear Research
1070 (CERN) is the largest scientific organization leading particle physics research. About
1071 13000 people in a broad range of roles including users, students, scientists, engineers,
1072 among others, contribute to the data taking and analysis, with the goal of unveiling
1073 the secrets of nature and revealing the fundamental structure of the universe. CERN
1074 is also the home of the Large Hadron Collider (LHC), the largest particle accelerator
1075 around the world, where protons (or heavy ions) traveling close to the speed of light,
1076 are made to collide. These collisions open a window to investigate how particles (and
1077 their constituents if they are composite) interact with each other, providing clues
1078 about the laws of nature. This chapter presents an overview of the LHC structure
1079 and operation. A detailed description of the CMS detector is offered, given that the
1080 data used in this thesis have been taken with this detector.

1081 2.2 The LHC

1082 With 27 km of circumference, the LHC is currently the most powerful circular accelerator
 1083 in the world. It is installed in the same tunnel where the Large Electron-Positron
 1084 (LEP) collider was located, taking advantage of the existing infrastructure. The LHC
 1085 is part of the CERN's accelerator complex composed of several successive accelerat-
 1086 ing stages before the particles are injected into the LHC ring where they reach their
 1087 maximum energy (see Figure 2.1).

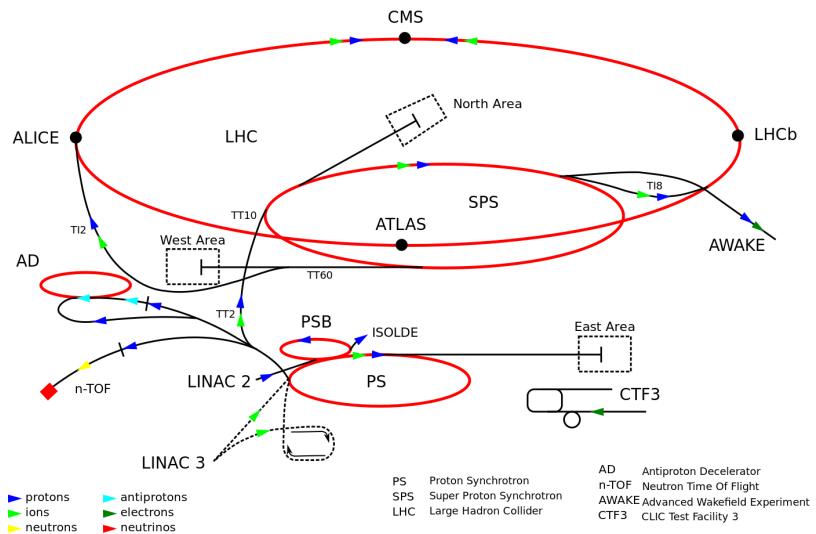


Figure 2.1: CERN accelerator complex. Blue arrows show the path followed by protons along the acceleration process [61].

1088 The LHC runs in three collision modes depending on the particles being acceler-
 1089 ated

- 1090 • Proton-Proton collisions (pp) for multiple physics experiments.
- 1091 • Lead-Lead collisions ($Pb-Pb$) for heavy ion experiments.
- 1092 • Proton-Lead collisions ($p-Pb$) for quark-gluon plasma experiments.

1093 In this thesis only pp collisions will be considered.

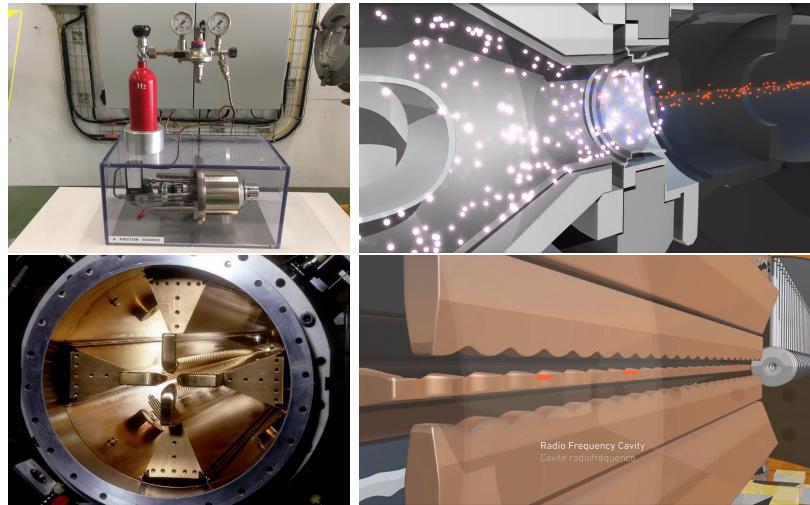


Figure 2.2: LHC protons source and the first acceleration stage. Top: the bottle contains hydrogen gas which is injected into the metal cylinder (white dots) to be broken down into electrons (blue dots) and protons (red dots); Bottom: the obtained protons are directed towards the radio frequency quadrupole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

1094 Collection of protons starts with hydrogen atoms taken from a bottle, containing
 1095 hydrogen gas, and injecting them in a metal cylinder; hydrogen atoms are broken
 1096 down into electrons and protons by an intense electric field (see Figure 2.2 top).
 1097 The resulting protons leave the metal cylinder towards a radio frequency quadrupole
 1098 (RFQ) that focus the beam, accelerates the protons and creates the packets of protons
 1099 called bunches. In the RFQ, an electric field is generated by a RF wave at a frequency
 1100 that matches the resonance frequency of the cavity where the electrodes are contained.
 1101 The beam of protons traveling on the RFQ axis experiences an alternating electric
 1102 field gradient that generates the focusing forces.

1103 In order to accelerate the protons, a longitudinal time-varying electric field com-
 1104 ponent is added to the system; it is done by giving the electrodes a sine-like profile as
 1105 shown in Figure 2.2 bottom. By matching the speed and phase of the protons with
 1106 the longitudinal electric field the bunching is performed; protons synchronized with

1107 the RFQ (synchronous protons) do not feel an accelerating force, but those protons in
 1108 the beam that have more (or less) energy than the synchronous proton (asynchronous
 1109 protons) will feel a decelerating (accelerating) force; therefore, asynchronous protons
 1110 will oscillate around the synchronous ones forming bunches of protons [63]. From the
 1111 RFQ protons emerge with energy 750 keV in bunches of about 1.15×10^{11} protons [64].

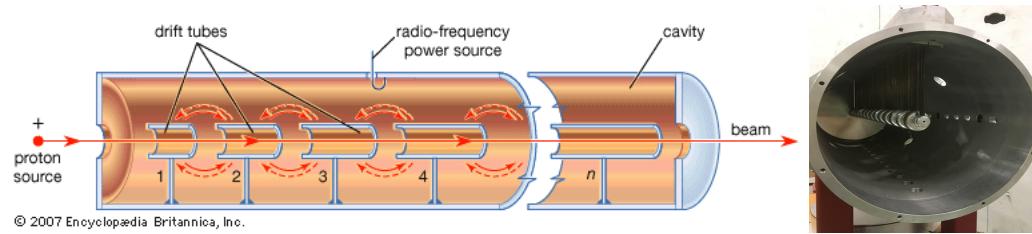


Figure 2.3: Left: drawing of the LINAC2 accelerating system at CERN. Electric fields generated by radio frequency (RF) create acceleration and deceleration zones inside the cavity; deceleration zones are blocked by drift tubes where quadrupole magnets focus the proton beam. Right: picture of a real RF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

1112 Proton bunches coming from the RFQ go to the linear accelerator 2 (LINAC2)
 1113 where they are accelerated to reach 50 MeV energy. In the LINAC2 stage, acceleration
 1114 is performed using electric fields generated by radio frequency which create zones
 1115 of acceleration and deceleration as shown in Figure 2.3. In the deceleration zones,
 1116 the electric field is blocked using drift tubes where protons are free to drift while
 1117 quadrupole magnets focus the beam.

1118 The beam coming from LINAC2 is injected into the proton synchrotron booster
 1119 (PSB) to reach 1.4 GeV in energy. The next acceleration is provided at the proton
 1120 synchrotron (PS) up to 26 GeV, followed by the injection into the super proton
 1121 synchrotron (SPS) where protons are accelerated to 450 GeV. Finally, protons are
 1122 injected into the LHC where they are accelerated to the target energy of 6.5 TeV.

1123 PSB, PS, SPS and LHC accelerate protons using the same RF acceleration tech-
 1124 nique described before.

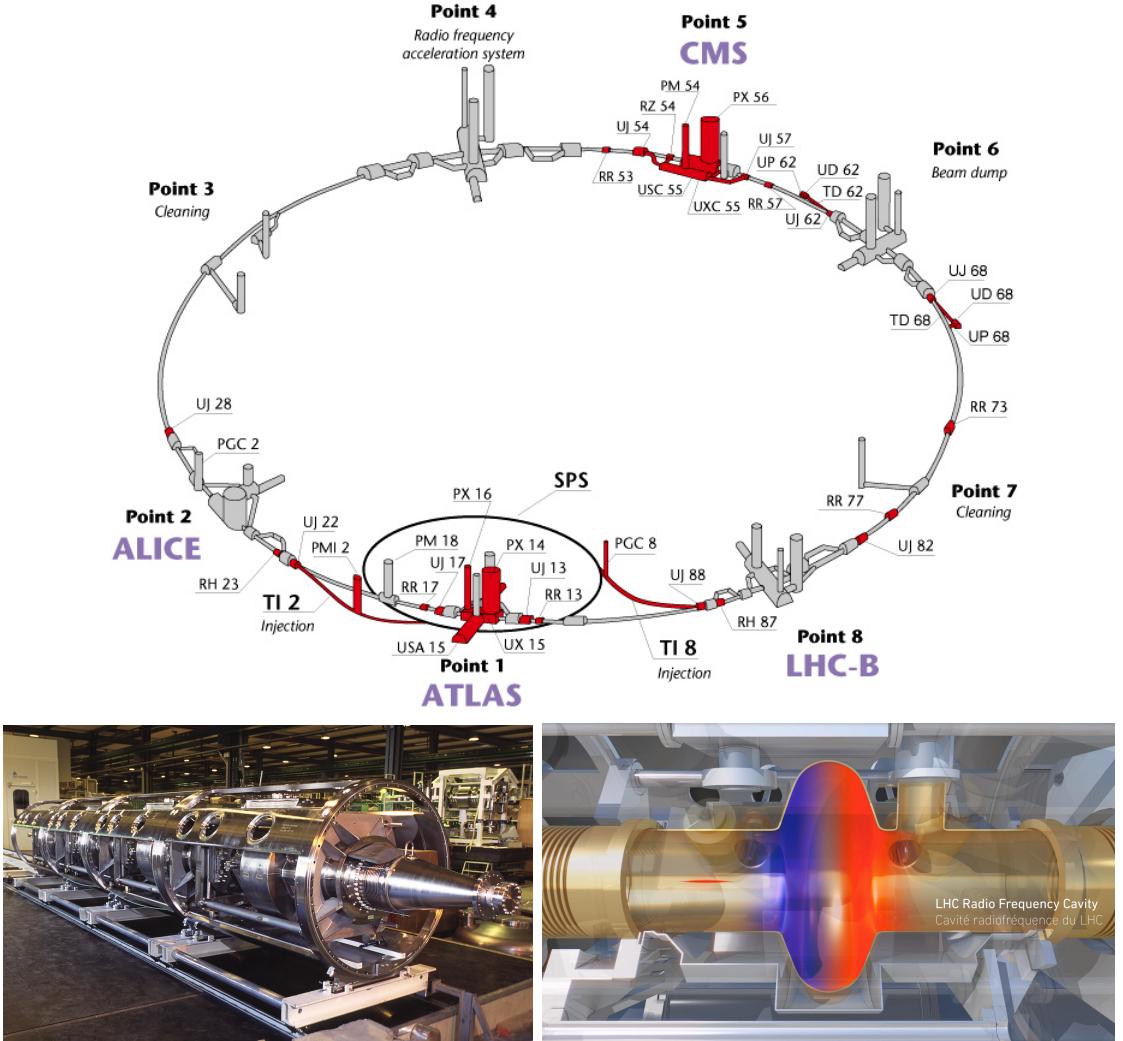


Figure 2.4: Top: LHC layout. The red zones indicate the infrastructure additions to the LEP installations, built to accommodate the ATLAS and CMS experiments which exceed the size of the former experiments located there [62]. Bottom: LHC RF cavities. A module (left picture) accommodates 4 cavities, each 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]

1125 The LHC has a system of 16 RF cavities located in the so-called point 4, as
 1126 shown in Figure 2.4 top, tuned at a frequency of 400 MHz. The bottom side of
 1127 Figure 2.4 shows a picture of a RF module composed of 4 RF cavities working in a
 1128 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

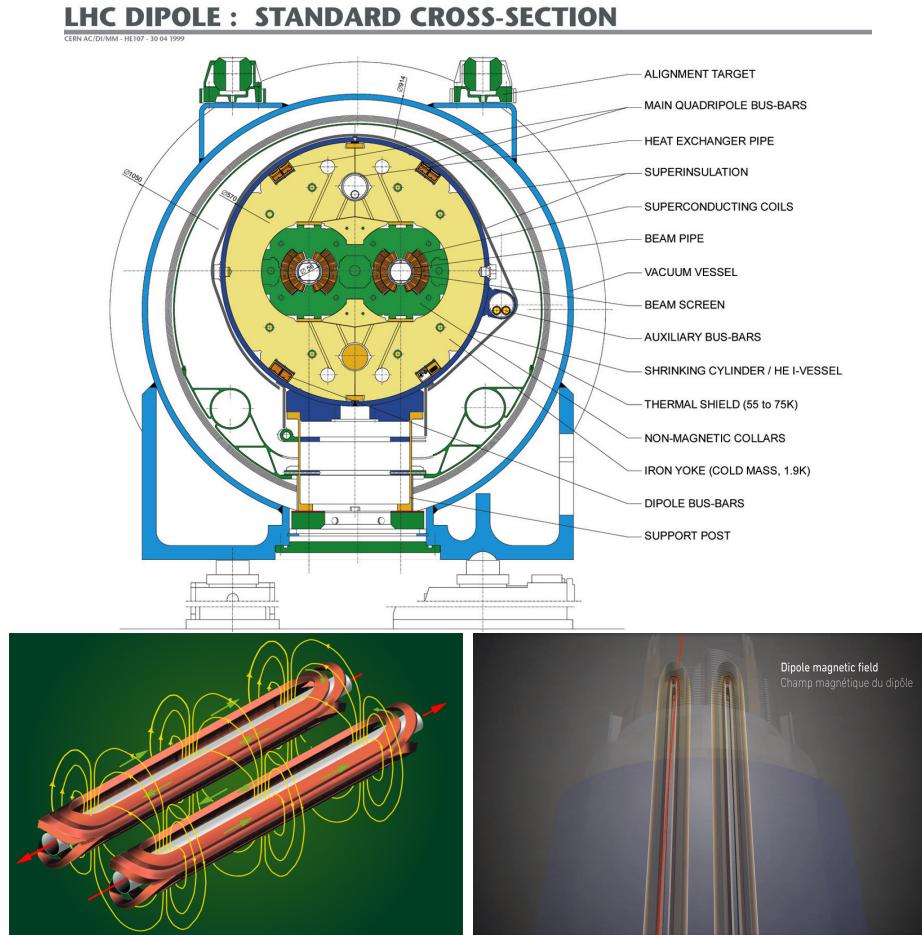


Figure 2.5: Top: LHC dipole magnet transverse view; cooling, shielding and mechanical support are indicated. Bottom left: Magnetic field generated by the dipole magnets; note that the direction of the field inside one beam pipe is opposite with respect to the other beam pipe which guarantee that both 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].

1152 magnetic field generated by the dipole magnets is shown on the bottom left side of
 1153 Figure 2.5. The bending effect of the magnetic field on the proton beam is shown on
 1154 the bottom right side of Figure 2.5. Note that the dipole magnets are not curved;
 1155 the arc section of the LHC ring is composed of straight dipole magnets of about 15
 1156 m. In total there are 1232 dipole magnets along the LHC ring.

1157 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 μm 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, σ_x and σ_y are the gaussian transverse sizes of the bunches. With the expected parameters, the LHC expected luminosity is about

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

$$n = 2808$$

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

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

1173

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

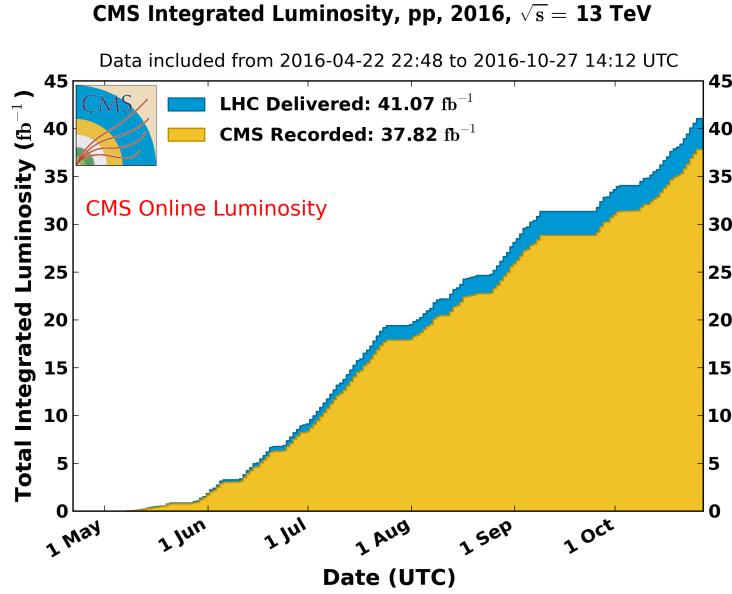


Figure 2.6: Integrated luminosity delivered by LHC and recorded by CMS during 2016. The difference between the delivered and the recorded luminosity is due to fails and issues occurred during the data taking in the CMS experiment [71].

1174 Luminosity is a fundamental aspect of LHC given that the bigger luminosity the
1175 bigger number of collisions, which means that for processes with a very small cross
1176 section the number of expected occurrences is increased and so the chances of being
1177 detected. The integrated luminosity, collected by the CMS experiment during 2016
1178 is shown in Figure 2.6; the data analyzed in this thesis corresponds to an integrated
1179 luminosity of 35.9 fb^{-1} at a center of mass-energy $\sqrt{s} = 13 \text{ TeV}$.

1180 One way to increase L is increasing the number of bunches in the beam. Cur-
1181 rently, the separation between two consecutive bunches in the beam is 7.5 m which
1182 corresponds to a time separation of 25 ns. In the full LHC ring the allowed number
1183 of bunches is $n = 27\text{km}/7.5\text{m} = 3600$; however, there are some gaps in the bunch pat-
1184 tern intended for preparing the dumping and injection of the beam, thus, the proton
1185 beams are composed of 2808 bunches.

1186 Once the proton beams reach the desired energy, they are brought to cross each

1187 other producing pp collisions. The bunch crossing happens in precise places where
 1188 the four LHC experiments are located, as seen in the top of Figure 2.7. In 2008 pp
 1189 collisions of $\sqrt{s} = 7$ TeV were performed; the energy was increased to 8 TeV in 2012
 1190 and to 13 TeV in 2015.

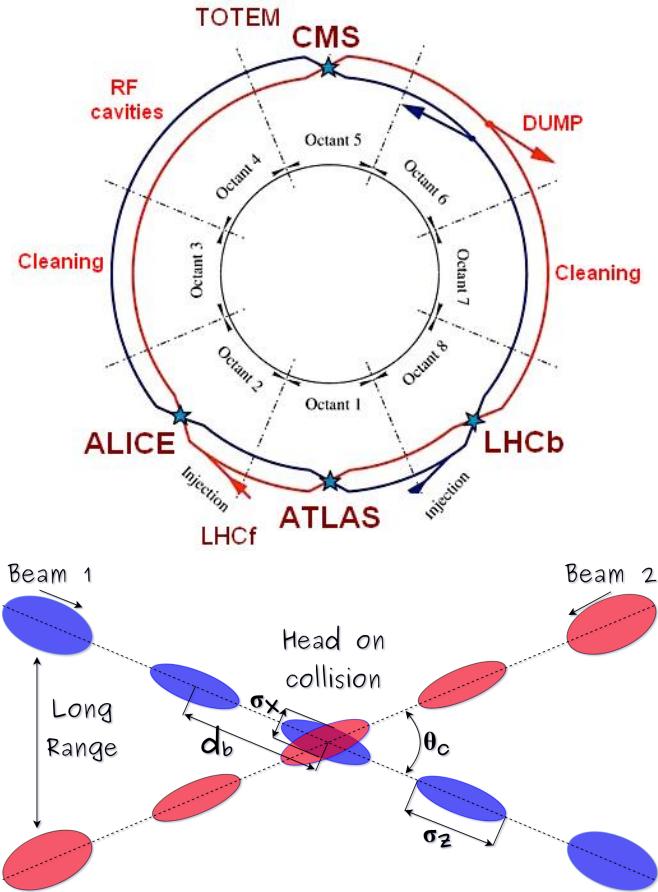


Figure 2.7: Top: LHC interaction points. Bunch crossing occurs where the LHC experiments are located [72]. Sections indicated as cleaning are dedicated to collimate the beam in order to protect the LHC ring from collisions with protons in very spreaded bunches. Bottom: bunch crossing scheme. Since the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

1191 The CMS and ATLAS experiments are multi-purpose experiments, hence, they
 1192 are enabled to explore physics in any of the LHC collision modes. LHCb experiment
 1193 is optimized to explore bottom quark physics, while ALICE is optimized for heavy

1194 ion collisions searches; TOTEM and LHCf are dedicated to forward physics studies;
 1195 MoEDAL (not indicated in the Figure) is intended for monopole or massive pseudo
 1196 stable particles searches.

1197 At the IP there are two interesting details that need to be addressed. The first
 1198 one is that the bunch crossing does not occur head-on but at a small crossing angle θ_c
 1199 (280 μ rad in CMS and ATLAS) as shown in the bottom side of Figure 2.7, affecting
 1200 the overlapping between bunches; the consequence is a reduction of about 17% in
 1201 the luminosity (represented by a factor not included in eqn. 2.2). The second one
 1202 is the occurrence of multiple pp collisions in the same bunch crossing; this effect is
 1203 called *pileup* (PU). A fairly simple estimation of the PU follows from estimating the
 1204 probability of collision between two protons, one from each of the bunches in the
 1205 course of collision; it depends roughly on the ratio of proton size and the cross section
 1206 of the bunch in the IP, i.e.,

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

1207 however, there are $N = 1.15 \times 10^{11}$ protons in a bunch, thus the estimated number of
 1208 collisions in a bunch crossing is

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

1209 about 20 of which are inelastic. A multiple pp collision event in a bunch crossing at
 1210 CMS is shown in Figure 2.8.

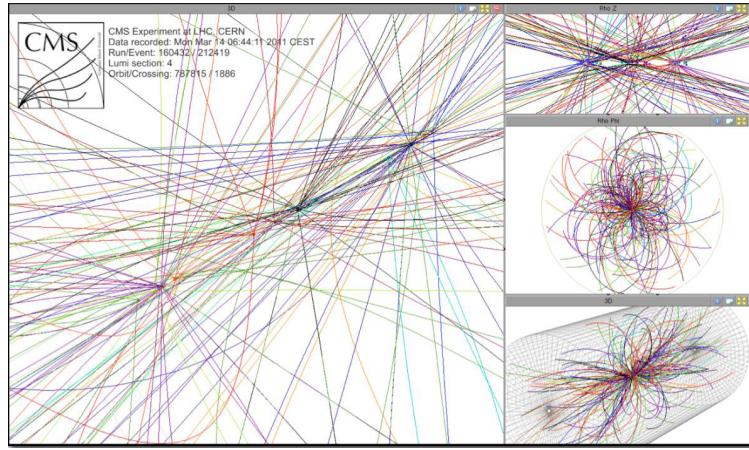


Figure 2.8: Multiple $p\bar{p}$ collision bunch crossing at CMS. [73].

1211 2.3 The CMS experiment

1212 CMS is a general-purpose detector designed to conduct research in a wide range
 1213 of physics from the standard model to new physics like extra dimensions and dark
 1214 matter. Located at Point 5 in the LHC layout as shown in Figure 2.4, CMS is
 1215 composed of several detection systems distributed in a cylindrical structure; in total,
 1216 CMS weights about 12500 tons in a very compact 21.6 m long and 14.6 m diameter
 1217 cylinder. It was built in 15 separate sections at the ground level and lowered to the
 1218 cavern individually to be assembled. A complete and detailed description of the CMS
 1219 detector and its components is given in Reference [74] on which this section is based.
 1220 Figure 2.9 shows the layout of the CMS detector. The detection system is composed
 1221 of (from the innermost to the outermost)

- 1222 • Pixel detector.
- 1223 • Silicon strip tracker.
- 1224 • Preshower detector.
- 1225 • Electromagnetic calorimeter.

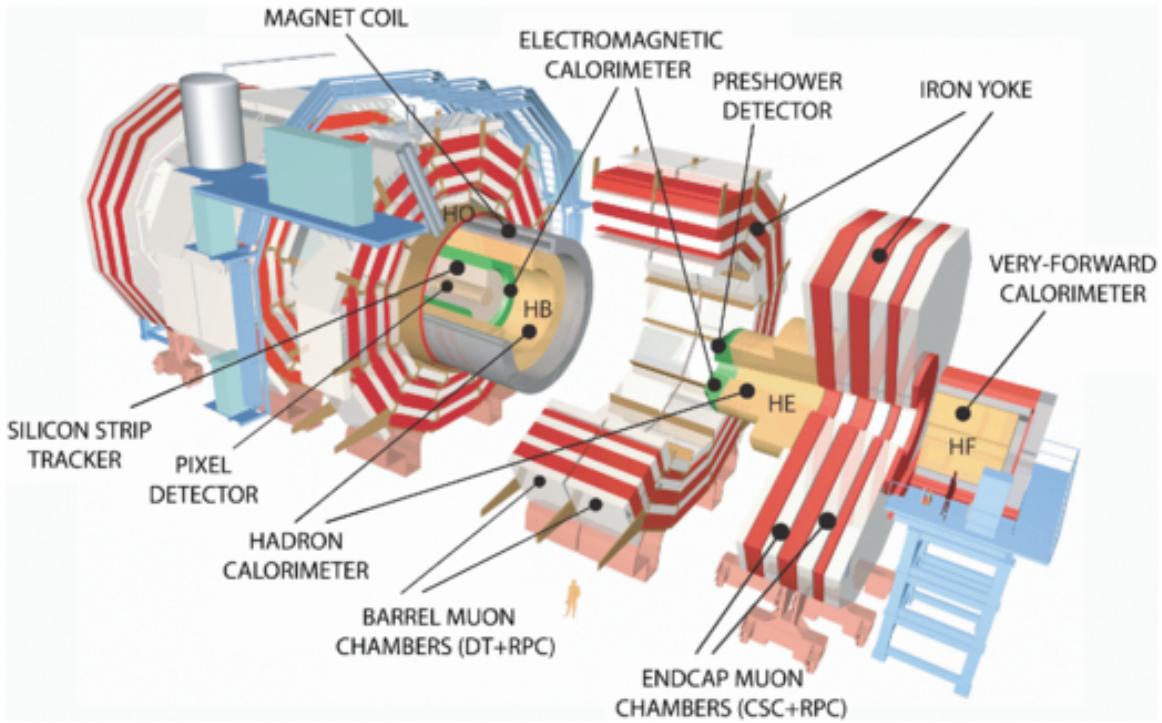


Figure 2.9: Layout of the CMS detector. The several subdetectors are indicated. The central region of the detector is referred as the barrel section while the endcaps are referred as the forward sections. [75].

1226 • Hadronic calorimeter.

1227 • Muon chambers (barrel and endcap)

1228 The central region of the detector is commonly referred as the barrel section while
 1229 the endcaps are referred as the forward sections of the detector; thus, each subdetector
 1230 is composed of a barrel section and a forward section.

1231 When a pp collision happens inside the CMS detector, many different particles are
 1232 produced, but only some of them live long enough to be detected; they are electrons,
 1233 photons, pions, kaons, protons, neutrons and muons; neutrinos are not detected by
 1234 the CMS detector. Thus, the CMS detector was designed to detect those particles and
 1235 measure their properties. Figure 2.10 shows a transverse slice of the CMS detector.
 1236 The silicon tracker (pixel detector + strip tracker) is capable to register the track of

1237 the charged particles traversing it, while calorimeters (electromagnetic and hadronic)
 1238 measure the energy of the particles that are absorbed by their materials. Considering
 1239 the detectable particles, mentioned above, emerging from the IP, a basic description
 1240 of the detection process is as follows.

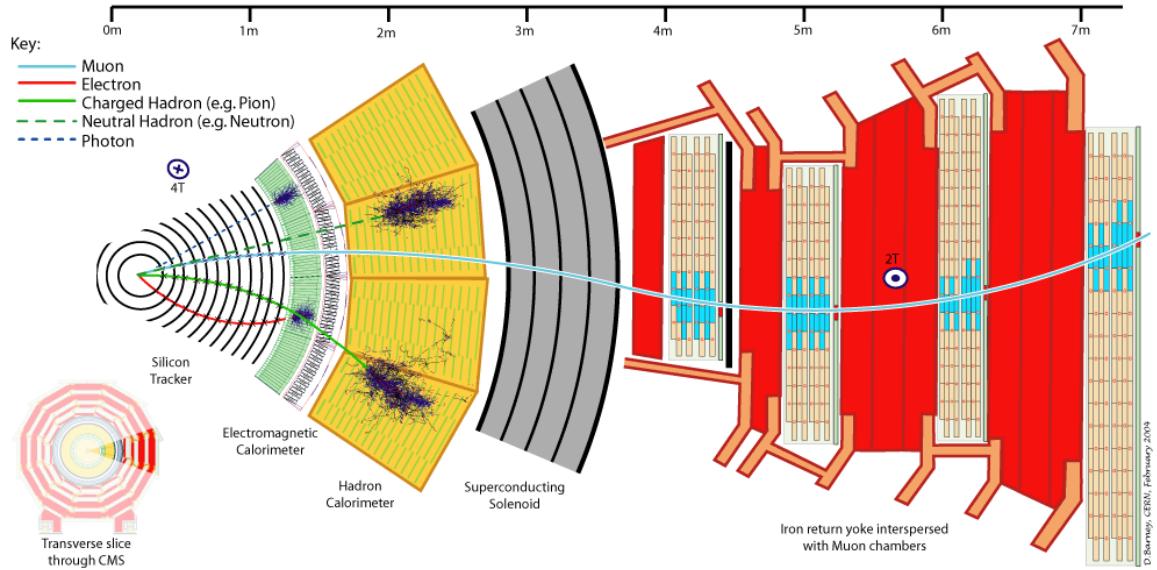


Figure 2.10: CMS detector transverse slice [76].

1241 A muon emerging from the IP, will create a track on the silicon tracker and on
 1242 the muon chambers. The design of the CMS detector is driven by the requirements
 1243 on the identification, momentum resolution and unambiguous charge determination
 1244 of the muons; therefore, a large bending power is provided by the solenoid magnet
 1245 made of superconducting cable capable of generating a 3.8 T magnetic field. The
 1246 muon track is bent twice since the magnetic field inside the solenoid is directed along
 1247 the z -direction but outside its direction is reversed. Muons interact very weakly with
 1248 the calorimeters, therefore, it is not absorbed but escape away from the detector.

1249 An electron emerging from the IP will create a track along the tracker which will
 1250 be bent due to the presence of the magnetic field, later, it will be absorbed in the
 1251 electromagnetic calorimeter where its energy is measured.

1252 A photon will not leave a track because it is neutral, but it will be absorbed in
 1253 the electromagnetic calorimeter.

1254 A neutral hadron, like the neutron, will not leave a track either but it will lose a
 1255 small amount of its energy during its passage through the electromagnetic calorimeter
 1256 and then it will be absorbed in the hadron calorimeter depositing the rest of its energy.

1257 A charged hadron, like the proton or π^\pm , will leave a curved track on the silicon
 1258 tracker, some of its energy in the electromagnetic calorimeter and finally will be
 1259 absorbed in the hadronic calorimeter.

1260 A more detailed description of each detection system will be presented in the
 1261 following sections.

1262 2.3.1 CMS coordinate system

1263 The coordinate system used by CMS is centered on the geometrical center of the
 1264 detector which is the nominal IP as shown in Figure 2.11¹. The z -axis is parallel
 1265 to the beam direction, while the Y -axis pointing vertically upward, and the X -axis
 1266 pointing radially inward toward the center of the LHC.

1267 In addition to the common cartesian and cylindrical coordinate systems, two co-
 1268 ordinates are of particular utility in particle physics: rapidity (y) and pseudorapidity
 1269 (η), defined in connection to the polar angle θ , energy and longitudinal momentum
 1270 component (momentum along the z -axis) according to

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

1271 Rapidity is related to the angle between the XY -plane and the direction in which
 1272 the products of a collision are emitted; it has the nice property that the difference

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

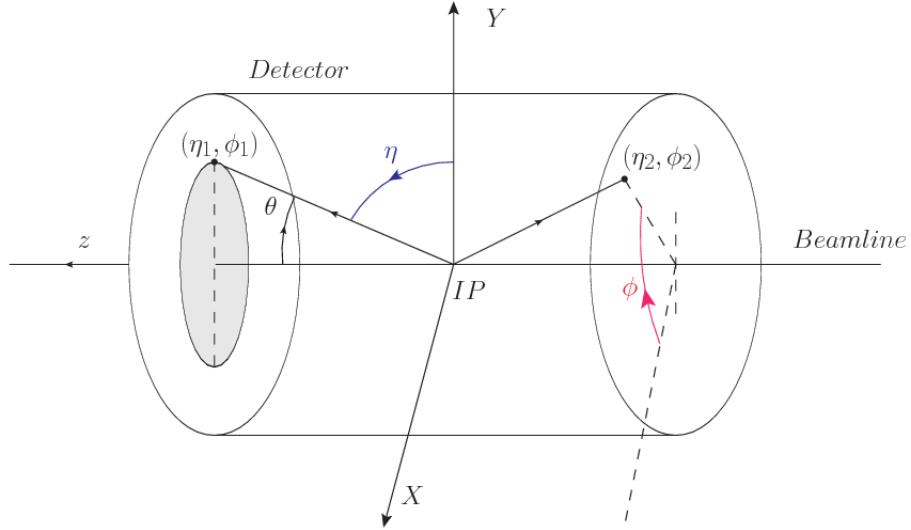


Figure 2.11: CMS detector coordinate system.

1273 between the rapidities of two particles is invariant with respect to Lorentz boosts
 1274 along the z -axis, hence, data analysis becomes more simple when based on rapid-
 1275 ity; however, it is not simple to measure the rapidity of highly relativistic particles,
 1276 as those produced after pp collisions. Under the highly relativistic motion approxi-
 1277 mation, y can be rewritten in terms of the polar angle, concluding that rapidity is
 1278 approximately equal to the pseudorapidity defined above, i.e., $y \approx \eta$. Note that η
 1279 is easier to measure than y given the direct relationship between the former and the
 1280 polar angle.

1281 The angular distance between two objects in the detector (ΔR) is commonly used
 1282 to judge the isolation of those object; it is defined in terms of their coordinates (η_1, ϕ_1) ,
 1283 (η_2, ϕ_2) as

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

1284 2.3.2 Tracking system

1285 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
 1286 precise reconstruction of the primary and secondary origins of the tracks (*vertices*) is
 1287 expected in an environment where, each 25 ns, the bunch crossing produces about 20
 1288 inelastic collisions and about 1000 particles.
 1289

1290 Physics requirements guiding the tracking system performance include the precise characterization of events involving gauge bosons, W and Z, and their leptonic
 1291 decays for which an efficient isolated lepton and photon reconstruction is of capital
 1292 importance, given that isolation is required to suppress background events to a level
 1293 that allows observations of interesting processes like Higgs boson decays or beyond
 1294 SM events.

1296 The ability to identify and reconstruct b -jets and B-hadrons within these jets is also
 1297 a fundamental requirement, achieved through the ability to reconstruct accurately
 1298 displaced vertices, given that b -jets are part of the signature of top quark physics, like
 1299 the one treated in this thesis.

1300 An schematic view of the CMS tracking system is shown in Figure 2.12

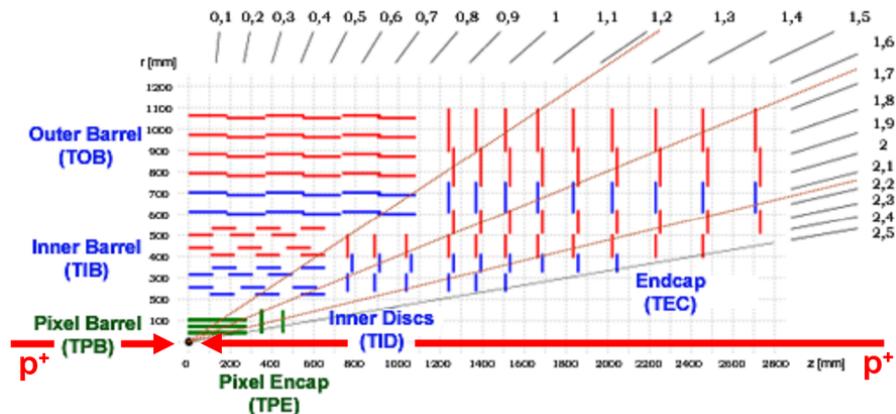


Figure 2.12: CMS tracking system schematic view [78].

1301 In order to satisfy these performance requirements, the tracking system uses two
 1302 different detector subsystems arranged in concentric cylindrical volumes, the pixel
 1303 detector and the silicon strip tracker; the pixel detector is located in the high particle
 1304 density region ($r < 20\text{cm}$) while the silicon strip tracker is located in the medium and
 1305 lower particle density regions $20\text{cm} < r < 116\text{cm}$.

1306 **Pixel detector**

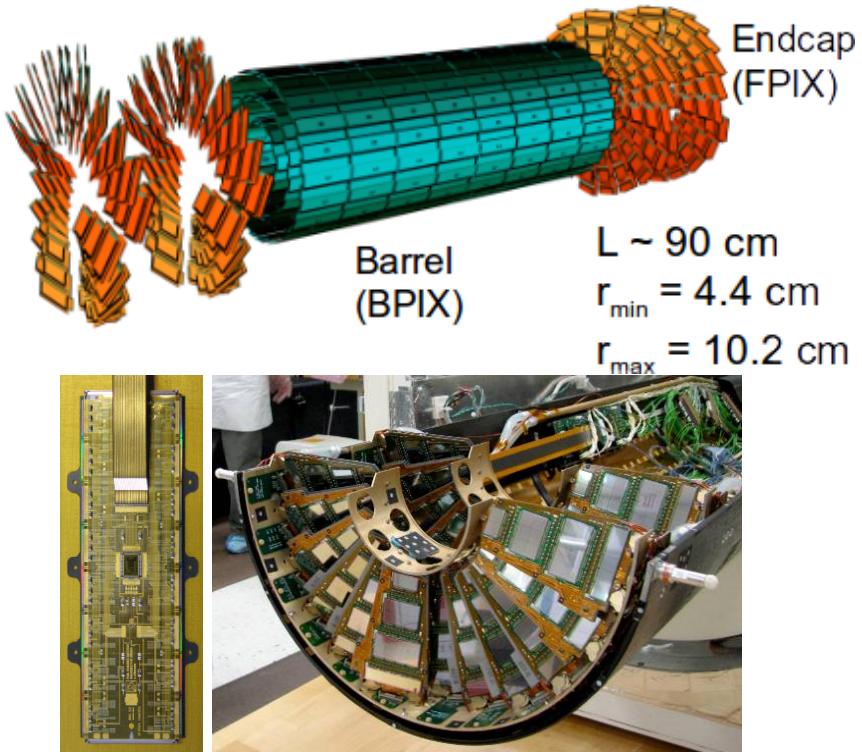


Figure 2.13: CMS pixel detector. Top: schematic view; Bottom: pictures of a barrel(BPIX) module(left) and forward modules(right) [74].

1307 The pixel detector was replaced during the 2016-2017 extended year-end technical
 1308 stop, due to the increasingly challenging operating conditions like the higher particle
 1309 flux and more radiation harsh environment, among others. The new one is responding
 1310 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

1337 blades in the turbine-like layout as shown in Figure 2.13 bottom left.

1338 2.3.3 Silicon strip tracker

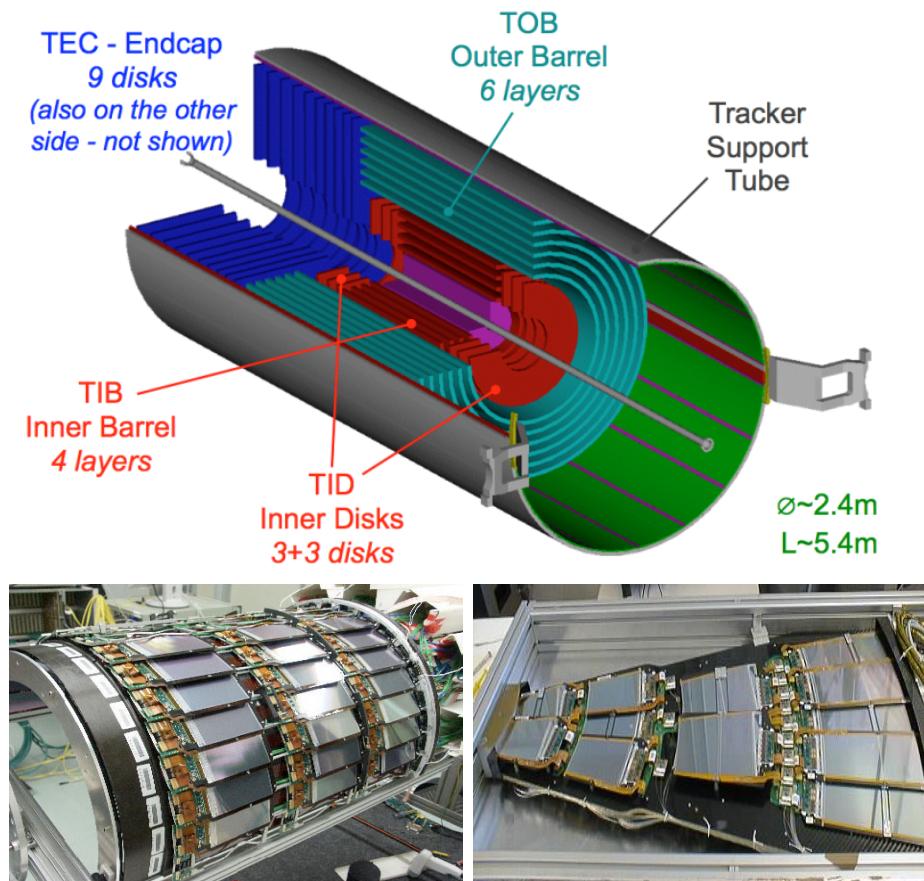


Figure 2.14: Top: CMS Silicon Strip Tracker (SST) schematic view. The SST is composed of the tracker inner barrel (TIB), the tracker inner disks (TID), the tracker outer barrel (TOB) and the tracker endcaps (TEC). Each part is made of silicon strip modules; the modules in blue represent two modules mounted 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].

1339 The silicon strip tracker (SST) is the second stage in the CMS tracking system.

1340 The top side of Figure 2.14 shows a schematic of the SST. The inner tracker region is

1341 composed of the tracker inner barrel (TIB) and the tracker inner disks (TID) covering

1342 the region $r < 55$ cm and $|z| < 118$ cm. The TIB is composed of 4 layers while the TID

1343 is composed of 3 disks at each end. The silicon sensors in the inner tracker are 320
 1344 μm thick, providing a resolution of about 13-38 μm in the $r\phi$ position measurement.

1345 The modules indicated in blue in the schematic view of Figure 2.14 are two mod-
 1346 ules mounted back-to-back and rotated in the plane of the module by a *stereo* angle
 1347 of 100 mrad; the hits from these two modules, known as *stereo hits*, are combined to
 1348 provide a measurement of the second coordinate (z in the barrel and r on the disks)
 1349 allowing the reconstruction of hit positions in 3-D.

1350 The outer tracker region is composed of the tracker outer barrel (TOB) and the
 1351 tracker endcaps (TEC). The six layers of the TOB offer coverage in the region $r > 55$
 1352 cm and $|z| < 118$ cm, while the 9 disks of the TEC cover the region $124 < |z| < 282$
 1353 cm. The resolution offered by the outer tracker is about 13-38 μm in the $r\phi$ position
 1354 measurement. The inner four TEC disks use silicon sensors 320 μm thick; those in
 1355 the TOB and the outer three TEC disks use silicon sensors of 500 μm thickness. The
 1356 silicon strips run parallel to the z -axis and the distance between strips varies from 80
 1357 μm in the inner TIB layers to 183 μm in the inner TOB layers; in the endcaps the
 1358 wedge-shaped sensors with radial strips, whose pitch range between 81 μm at small
 1359 radii and 205 μm at large radii.

1360 The whole SST has 15148 silicon modules, 9.3 million silicon strips and cover a
 1361 total active area of about 198 m^2 .

1362 **2.3.4 Electromagnetic calorimeter**

1363 The CMS electromagnetic calorimeter (ECAL) is designed to measure the energy of
 1364 electrons and photons. It is composed of 75848 lead tungstate crystals which have a
 1365 short radiation length (0.89 cm) and fast response, since 80% of the light is emitted
 1366 within 25 ns; however, they are combined with Avalanche photodiodes (APDs) as

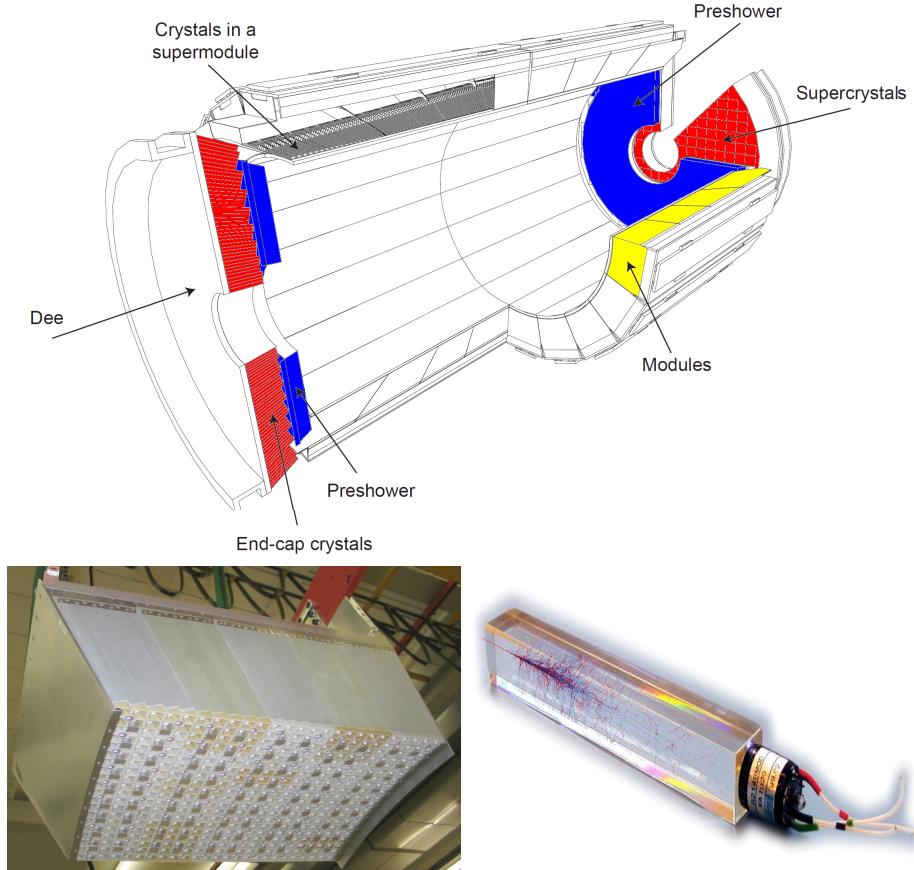


Figure 2.15: Top: CMS ECAL schematic view. Bottom: Module equipped with the crystals (left); ECAL crystal(right) with an artistic representation of an electromagnetic shower [74].

1367 photodetectors given that crystals themselves have a low light yield ($30\gamma/\text{MeV}$). A
 1368 schematic view of the ECAL is shown in Figure 2.15.

1369 Energy is measured when electrons and photons are absorbed by the crystals
 1370 which generates an electromagnetic *shower*, as seen in bottom right picture of the
 1371 Figure 2.15; the shower is seen as a *cluster* of energy which depending on the amount
 1372 of energy deposited can involve several crystals. The ECAL barrel (EB) covers the
 1373 region $|\eta| < 1.479$, using crystals of depth of 23 cm and $2.2 \times 2.2 \text{ cm}^2$ transverse
 1374 section; the ECAL endcap (EE) covers the region $1.479 < |\eta| < 3.0$ using crystals of
 1375 depth 22 cm and transverse section of $2.86 \times 2.86 \text{ cm}^2$; the photodetectors used are

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

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

2.3.5 Hadronic calorimeter

Hadrons are not absorbed by the ECAL² but by the hadron calorimeter (HCAL), which is made of a combination of alternating brass absorber layers and silicon photomultiplier(SiPM) layers; therefore, particles passing through the scintillator material produce showers, as in the ECAL, as a result of the inelastic scattering of the hadrons with the detector material. Since the particles are not absorbed in the scintillator, their energy is sampled; therefore the total energy is not measured but estimated from the energy clusters, which reduces the resolution of the detector. Brass was chosen as the absorber material due to its short interaction length ($\lambda_I = 16.42\text{cm}$) and its non-magnetivity. Figure 2.16 shows a schematic view of the CMS HCAL.

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

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

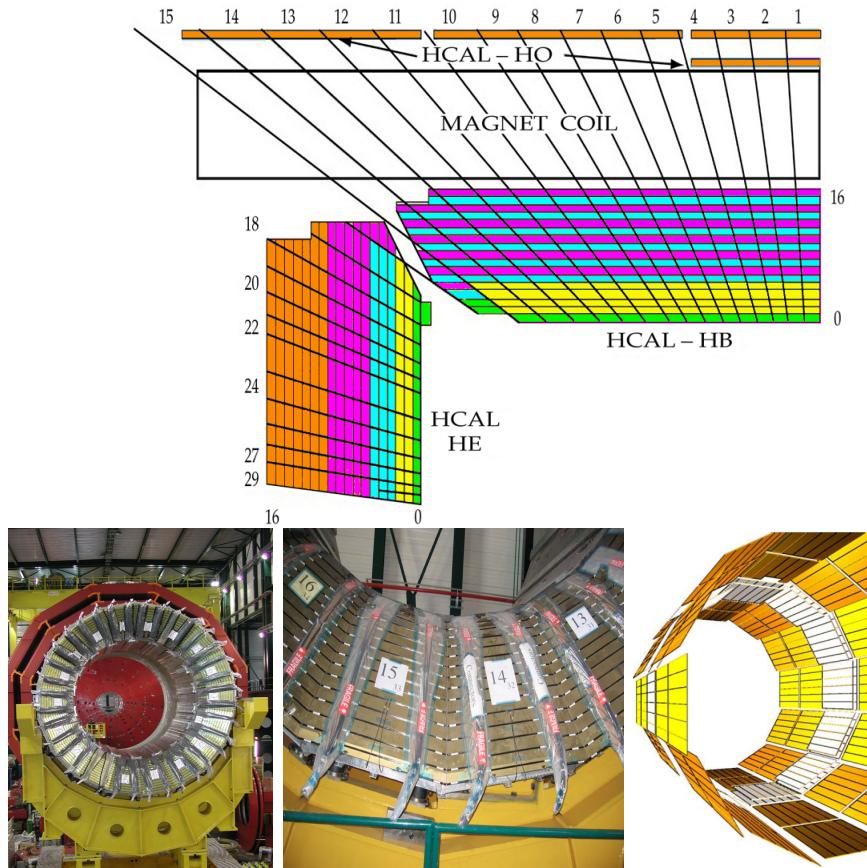


Figure 2.16: Top: CMS HCAL schematic view, the colors indicate the layers that are grouped into the same readout channels. Bottom: picture of a section of the HB; the absorber material is the golden region and scintillators are placed in between the absorber material (left and center). Schematic view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

1400 purpose of measure the energy tails of particles passing through the HB and the
 1401 magnet (see Figure 2.16 top and bottom right).

1402 **2.3.6 Superconducting solenoid magnet**

1403 The superconducting magnet installed in the CMS detector is designed to provide
 1404 an intense and highly uniform magnetic field in the central part of the detector.
 1405 In fact, the tracking system takes advantage of the bending power of the magnetic
 1406 field to measure with precision the momentum of the particles that traverse it; the

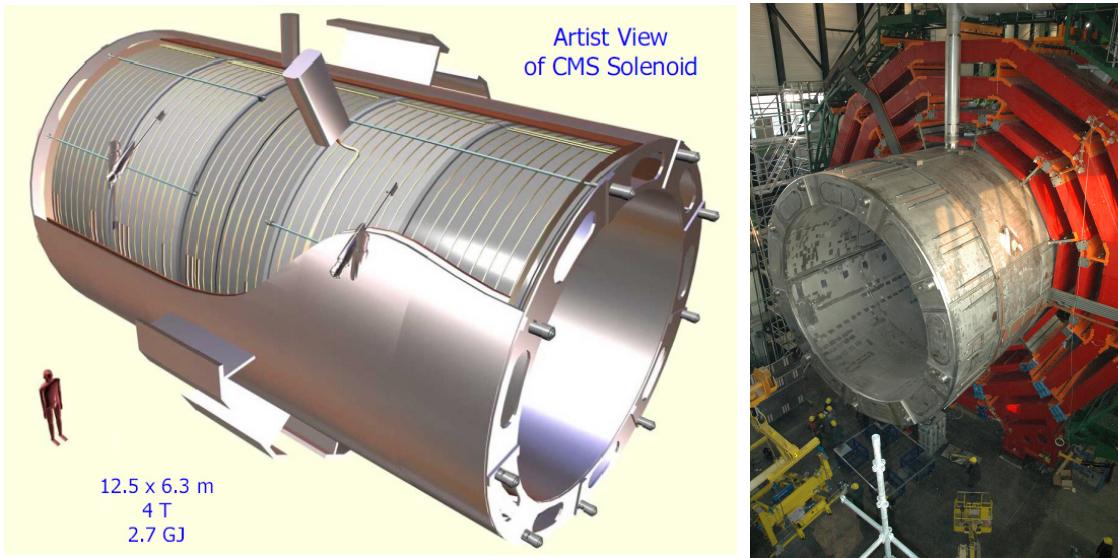


Figure 2.17: Artistic representation of the CMS solenoid magnet(left). The magnet is supported on an iron yoke (right) which also serves as the house of the muon detector and as mechanical support for the whole CMS detector [77].

1407 unambiguous determination of the sign for high momentum muons was a driving
 1408 principle during the design of the magnet. The magnet has a diameter of 6.3 m, a
 1409 length of 12.5 m and a cold mass of 220 t; the generated magnetic field reaches a
 1410 strength of 3.8T. Since it is made of Ni-Tb superconducting cable it has to operate at
 1411 a temperature of 4.7 K by using a helium cryogenic system; the current circulating in
 1412 the cables reaches 18800 A under normal running conditions. The left side of Figure
 1413 2.17 shows an artistic view of the CMS magnet, while the right side shows a transverse
 1414 view of the cold mass where the winding structure is visible.

1415 The yoke (see Figure 2.17), composed of 5 barrel wheels and 6 endcap disks made
 1416 of iron, serves not only as the media for magnetic flux return but also provides housing
 1417 for the muon detector system and structural stability to the full detector.

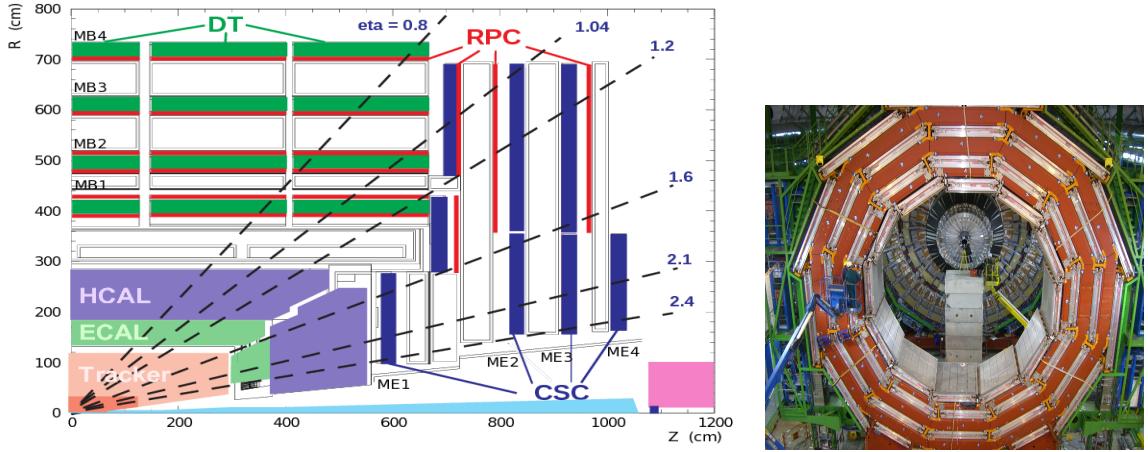


Figure 2.18: Left: CMS muon system schematic view; Right: one of the yoke rings with the muon DTs and RPCs installed; in the back it is possible to see the muon endcap [85].

1418 2.3.7 Muon system

1419 Muons are the only charged particles able to pass through all the CMS detector due
 1420 to their low ionization energy loss; thus, muons can be separated easily from the
 1421 high amount of particles produced in a pp collision. Also, muons are expected to be
 1422 produced in the decay of several new particles; therefore, good detection of muons
 1423 was one of the leading principles when designing the CMS detector.

1424 The CMS muon detection system (muon spectrometer) is embedded in the return
 1425 yoke as seen in Figure 2.18. It is composed of three different detector types, the drift
 1426 tube chambers (DT), cathode strip chambers (CSC), and resistive plate chambers
 1427 (RPC); DT are located in the central region $\eta < 1.2$ arranged in four layers of drift
 1428 chambers filled with an Ar/CO₂ gas mixture.

1429 The muon endcaps are made of CSCs covering the region $\eta < 2.4$ and filled with
 1430 a mixture of Ar/CO₂/CF₄. The reason behind using a different detector type lies on
 1431 the different conditions in the forward region like the higher muon rate and higher
 1432 residual magnetic field compared to the central region.

1433 The third type of detector used in the muon system is a set of four disks of RPCs

1434 working in avalanche mode. The RPCs provide good spatial and time resolutions. The
 1435 track of high- p_T muon candidates is built combining information from the tracking
 1436 system and the signal from up to six RPCs and four DT chambers.

1437 The muon tracks are reconstructed from the hits in the several layers of the muon
 1438 system.

1439 **2.3.8 CMS trigger system**

1440 CMS expects pp collisions every 25 ns, i.e., an interaction rate of 40 MHz for which
 1441 it is not possible to store the recorded data in full. In order to handle this high event
 1442 rate data, an online event selection, known as triggering, is performed; triggering
 1443 reduces the event rate to 100 Hz for storage and further offline analysis.

1444 The trigger system starts with a reduction of the event rate to 100 kHz in the
 1445 so-called *the level 1 trigger* (L1). L1 is based on dedicated programmable hardware
 1446 like Field Programmable Gate Arrays (FPGAs) and Application Specific Integrated
 1447 Circuits (ASICs), partly located in the detector itself; another portion is located in
 1448 the CMS underground cavern. Hit pattern information from the muon chambers
 1449 and the energy deposits in the calorimeter are used to decide if an event is accepted
 1450 or rejected, according to selection requirements previously defined, which reflect the
 1451 interesting physics processes. Figure 2.19 shows the L1 trigger architecture.

1452 The second stage in the trigger system is called *the high-level trigger* (HLT); events
 1453 accepted by L1 are passed to HLT in order to make an initial reconstruction of them.
 1454 HLT is software based and runs on a dedicated server farm, using selection algorithms
 1455 and high-level object definitions; the event rate at HLT is reduced to 100 Hz. The
 1456 first HLT stage takes information from the muon detectors and the calorimeters to
 1457 make the initial object reconstruction; in the next HLT stage, information from the

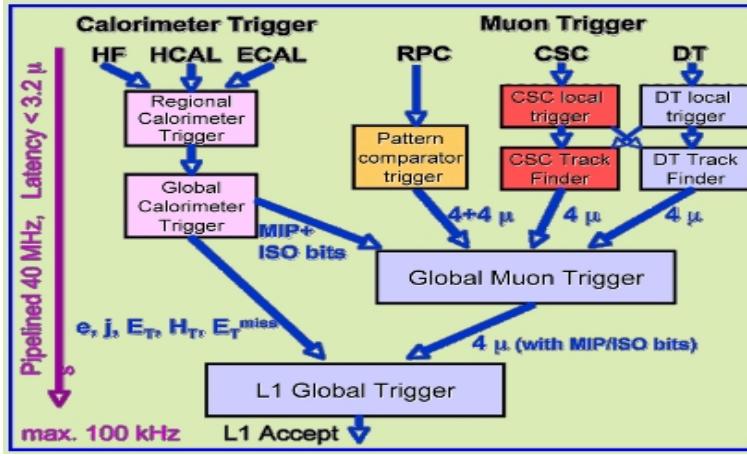


Figure 2.19: CMS Level-1 trigger architecture [86].

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, τ 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

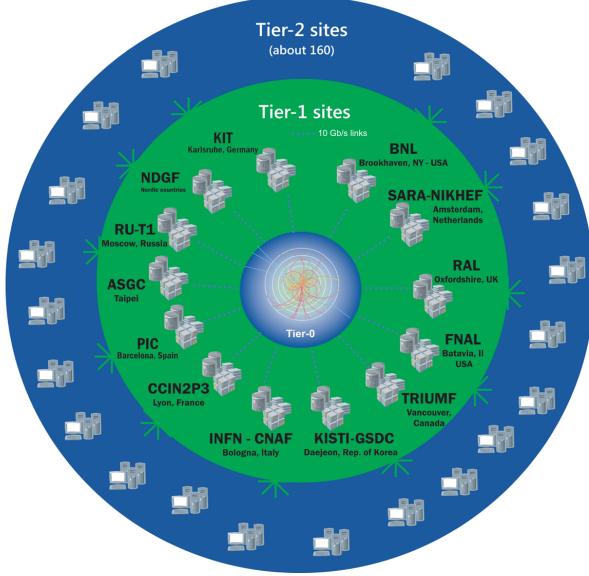


Figure 2.20: WLCG structure. The primary computer centers (Tier-0) are located at CERN (data center) and at the Wigner datacenter in Budapest. Tier-1 is composed of 13 centers and Tier-2 is composed of about 160 centers. [87].

1474 that distributed environment. WLCG is a tiered structure connecting computing
 1475 centers around the world, which provides the necessary storage and computing facil-
 1476 ties. The primary computing centers of the WLCG are located at the CERN and
 1477 the Wigner datacenter in Budapest and are known as Tier-0 as shown in Figure 2.20.
 1478 The main responsibilities for each tier level are [87]

- 1479 • **Tier-0:** initial reconstruction of recorded events and storage of the resulting
 1480 datasets, the distribution of raw data to the Tier-1 centers.
- 1481 • **Tier-1:** provide storage capacity, support for the Grid, safe-keeping of a pro-
 1482 portional share of raw and reconstructed data, large-scale reprocessing and safe-
 1483 keeping of corresponding output, generation of simulated events, distribution
 1484 of data to Tier 2s, safe-keeping of a share of simulated data produced at these
 1485 Tier 2s.
- 1486 • **Tier-2:** store sufficient data and provide adequate computing power for spe-

1487 cific analysis tasks and proportional share of simulated event production and
1488 reconstruction.

1489 Aside from the general computing strategy to manage the huge amount of data
1490 produced by experiments, CMS uses a software framework to perform a variety of
1491 processing, selection and analysis tasks. The central concept of the CMS data model
1492 referred to as *event data model* (EDM) is the *Event*; therefore, an event is the unit
1493 that contains the information from a single bunch crossing, any data derived from
1494 that information like the reconstructed objects, and the details of the derivation.

1495 Events are passed as the input to the *physics modules* that obtain information
1496 from them and create new information; for instance, *event data producers* add new
1497 data into the events, *analyzers* produce an information summary from an event set,
1498 *filters* perform selection and triggering.

1499 CMS uses several event formats with different levels of detail and precision

1500 • **Raw format:** events in this format contain the full recorded information from
1501 the detector as well as trigger decision and other metadata. An extended version
1502 of raw data is used to store information from the CMS Monte Carlo simulation
1503 tools (see Chapter 3). Raw data are stored permanently, occupying about
1504 2MB/event

1505 • **RECO format:** events in this format correspond to raw data that have been
1506 submitted to reconstruction algorithms like primary and secondary vertex re-
1507 construction, particle ID, and track finding. RECO events contain physics ob-
1508 jects and all the information used to reconstruct them; average size is about 0.5
1509 MB/event.

- 1510 • **AOD format:** Analysis Object Data (AOD) is the data format used in the
 1511 physics analyses given that it contains the parameters describing the high-level
 1512 physics objects in addition to enough information to allow a kinematic refitting if
 1513 needed. AOD events are filtered versions of the RECO events to which skimming
 1514 or other filtering have been applied, hence AOD events are subsets of RECO
 1515 events. Requires about 100 kB/event.
- 1516 • **Non-event data** are data needed to interpret and reconstruct events. Some
 1517 of the non-event data used by CMS contains information about the detector
 1518 contraction and condition data like calibrations, alignment, and detector status.

1519 Figure 2.21 shows the data flow scheme between CMS detector and tiers.

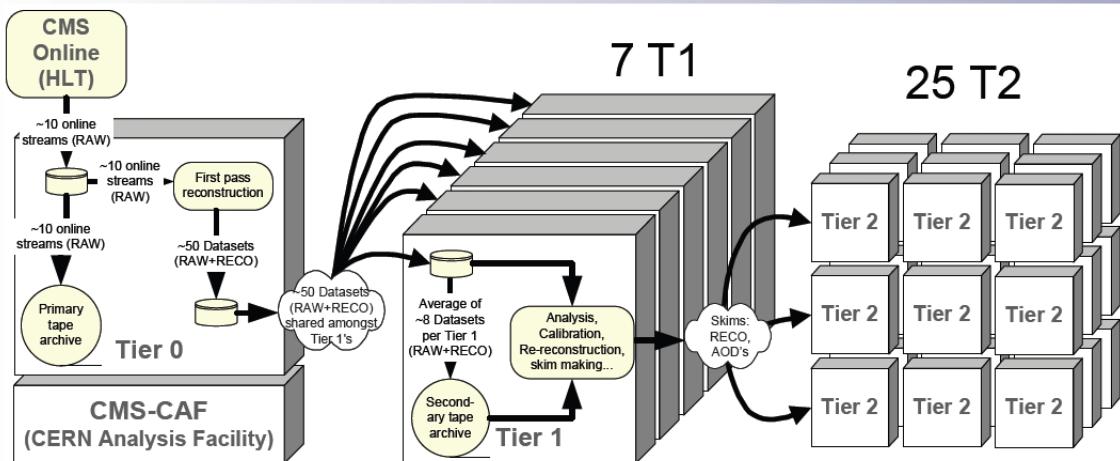


Figure 2.21: Data flow from CMS detector through tiers.

1520 The whole collection of software built as a framework is referred to as *CMSSW*. This
 1521 framework provides the services needed by the simulation, calibration and alignment,
 1522 and reconstruction modules that process event data, so that physicists can perform
 1523 analysis. The CMSSW event processing model is composed of one executable, called
 1524 `cmsRun`, and several plug-in modules which contains all the tools (calibration, recon-

1525 struction algorithms) needed to process an event. The same executable is used for
1526 both detector data and Monte Carlo simulations [88].

1527 **Chapter 3**

1528 **Event generation, simulation and
1529 reconstruction**

1530 The process of analyzing data recorded by the CMS experiment involves several stages
1531 where the data are processed in order to interpret the information provided by all
1532 the detection systems; in those stages, the particles produced after the pp collision
1533 are identified by reconstructing their trajectories and measuring their features. In
1534 addition, the SM provides a set of predictions that have to be compared with the
1535 experimental results; however, in most of the cases, theoretical predictions are not
1536 directly comparable to experimental results due to the diverse source of uncertainties
1537 introduced by the experimental setup and theoretical approximations, among others.

1538 The strategy to face these conditions consists in using statistical methods imple-
1539 mented in computational algorithms to produce numerical results that can be con-
1540 trasted with the experimental results. These computational algorithms are commonly
1541 known as Monte Carlo (MC) methods and, in the case of particle physics, they are
1542 designed to apply the SM rules and produce predictions about the physical observ-
1543 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

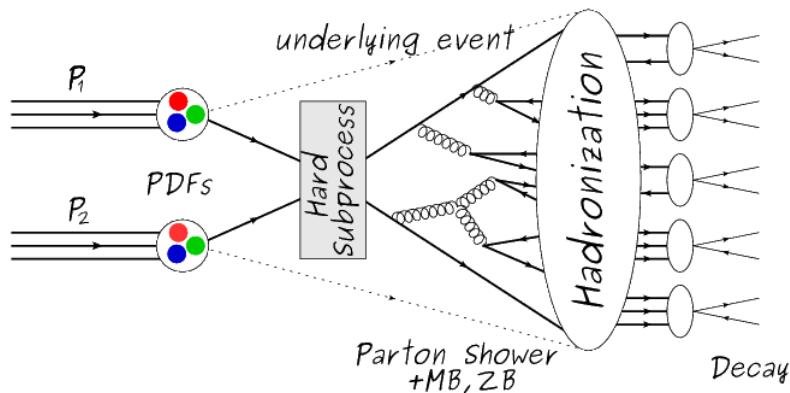


Figure 3.1: Event generation process. The actual interaction is generated in the hard subprocess. The parton shower describes the evolution of the partons from the hard subprocess. Modified from Reference [90].

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.

1558 Generation starts by taking into account the PDFs of the incoming particles.
 1559 Event generators offer the option to chose from several PDF sets depending on the
 1560 particular process under simulation¹; in the following, pp collisions will be consid-
 1561 ered. The *hard subprocess* describes the actual interaction between partons from the
 1562 incoming protons; it is represented by the matrix element connecting the initial and
 1563 final states of the interaction. Normally, the matrix element can be written as a
 1564 sum over Feynman diagrams and consider interferences between terms in the sum-
 1565 mation. During the generation of the hard subprocess, the production cross section
 1566 is calculated.

1567 The order to which the cross section is calculated depends on the order of the Feyn-
 1568 man diagrams involved in the calculation; therefore, radiative corrections are included
 1569 by considering a higher order Feynman diagrams where QCD radiation dominates.
 1570 Currently, cross sections calculated to LO do not offer a satisfactory description of the
 1571 processes, i.e., the results are only reliable for the shape of distributions; therefore,
 1572 NLO calculations have to be performed with the implication that the computing time
 1573 needed is highly increased.

1574 The final parton content of the hard subprocess is subjected to the *parton shower*
 1575 which generates the gluon radiation. Parton shower evolves the partons, i.e., glouns
 1576 split into quark-antiquark pairs and quarks with enough energy radiate gluons giv-
 1577 ing rise to further parton multiplication, following the DGLAP (Dokshitzer-Gribov-
 1578 Lipatov-Altarelli-Parisi) equations. Showering continues until the energy scale is low
 1579 enough to reach the non-perturbative limit.

1580 In the simulation of LHC processes that involve b quarks, like the single top quark
 1581 or Higgs associated production, it is needed to consider that the b quark is heavier
 1582 than the proton; hence, the QCD interaction description is made in two different

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

1583 schemes [95]

- 1584 • four-flavor (4F) scheme. b quarks appear only in the final state because they
 1585 are heavier than the proton and therefore they can be produced only from the
 1586 splitting of a gluon into pairs or singly in association with a t quark in high
 1587 energy-scale interactions; furthermore, during the simulation, the b -PDFs are set
 1588 to zero. Calculations in this scheme are more complicated due to the presence
 1589 of the second b quark but the full kinematics is considered already at LO and
 1590 therefore the accuracy of the description is better.

- 1591 • five-flavor (5F) scheme. b quarks are considered massless, therefore they can
 1592 appear in both initial and final states since they can now be part of the proton;
 1593 thus, during the simulation b -PDFs are not set to zero. In this scheme, calcu-
 1594 lations are simpler than in the 4F scheme and possible logarithmic divergences
 1595 are absorbed by the PDFs through the DGLAP evolution.

1596 In this thesis, the tHq events are generated using the 4F scheme in order to reduce
 1597 uncertainties, while the tHW events are generated using the 5F scheme to eliminate
 1598 LO interference with $t\bar{t}H$ process [48].

1599 Partons involved in the pp collision are the focus of the simulation, however, the
 1600 rest of the partons inside the incoming protons are also affected because the remnants
 1601 are colored objects; also, multiple parton interactions can occur. The hadronization
 1602 of the remnants and multiple parton interactions are known as *underlying event* and
 1603 it has to be included in the simulation. In addition, multiple pp collisions in the same
 1604 bunch crossing (pile-up mentioned in 2.2) occurs, actually in two forms

- 1605 • *in-time PU* which refers to multiple pp collision in the bunch crossing but that
 1606 are not considered as primary vertices.

1607 • *Out-of-time PU* which refers to overlapping pp collisions from consecutive bunch
 1608 crossings; this can occur due to the time-delays in the detection systems where
 1609 information from one bunch crossing is assigned to the next or previous one.

1610 While the underlying event effects are included in generation using generator-
 1611 specific tools, PU effects are added to the generation by overlaying Minimum-bias (MB)
 1612 and Zero-bias (ZB) events to the generated events. MB events are inelastic events
 1613 selected by using a loose trigger with as little bias as possible, therefore accepting a
 1614 large fraction of the overall inelastic event; ZB events correspond to random events
 1615 recorded by the detector when collisions are likely. MB models in-time PU and ZB
 1616 models out-of-time PU.

1617 The next step in the generation process is called *hadronization*. Since particles
 1618 with a net color charge are not allowed to exits isolated, they have to recombine
 1619 to form bound states. This is precisely the process by which the partons resulting
 1620 from the parton shower arrange themselves as color singlets to form hadrons. At
 1621 this step, the energy-scale is low and the strong coupling constant is large, therefore
 1622 hadronization process is non-perturbative and the evolution of the partons is described
 1623 using phenomenological models. Most of the baryons and mesons produced in the
 1624 hadronization are unstable and hence they will decay in the detector.

1625 The last step in the generation process corresponds to the decay of the unstable
 1626 particles generated during hadronization; it is also simulated in the hadronization
 1627 step, based on the known branching ratios.

1628 **3.2 Monte Carlo Event Generators.**

1629 The event generation described in the previous section has been implemented in
 1630 several software packages for which a brief description is given.

- 1631 • **PYTHIA 8.** It is a program designed to perform the generation of high energy
 1632 physics events which describes the collisions between particles such as electrons
 1633 and protons. Several theories and models are implemented in it, in order to
 1634 describe physical aspects like hard and soft interaction, parton distributions,
 1635 initial and final-state parton showers, multiple parton interactions, beam rem-
 1636 nants, hadronization² and particle decay. Thanks to extensive testing, several
 1637 optimized parametrizations, known as *tunings*, have been defined in order to
 1638 improve the description of actual collisions to a high degree of precision; for
 1639 analysis at $\sqrt{s} = 13$ TeV, the underline event CUETP8M1 tune is employed [97].
 1640 The calculation of the matrix element is performed at LO which is not enough
 1641 for the current required level of precision; therefore, pythia is often used for
 1642 parton shower, hadronization and decays, while other event generators are used
 1643 to generate the matrix element at NLO.
- 1644 • **MadGraph5_aMC@NLO.** MadGraph is a matrix element generator which
 1645 calculates the amplitudes for all contributing Feynman diagrams of a given
 1646 process but does not provide a parton shower while MC@NLO incorporates
 1647 NLO QCD matrix elements consistently into a parton shower framework; thus,
 1648 MadGraph5_aMC@NLO, as a merger of the two event generators MadGraph5
 1649 and aMC@NLO, is an event generator capable to calculate tree-level and NLO
 1650 cross sections and perform the matching of those with the parton shower. It is
 1651 one of the most frequently used matrix element generators; however, it has the
 1652 particular feature of the presence of negative event weights which reduce the
 1653 number of events used to reproduce the properties of the objects generated [98].
- 1654 • **POWHEG.** It is an NLO matrix element generator where the hardest emis-

² based in the Lund string model [96]

1655 sion of color charged particles is generated in such a way that the negative event
 1656 weights issue of MadGraph5_aMC@NLO is overcome; however, the method re-
 1657 quires an interface with p_T -ordered parton shower or a parton shower generator
 1658 where this highest emission can be vetoed in order to avoid double counting of
 1659 this highest-energetic emission. PYTHIA is a commonly matched to POWHEG
 1660 event generator [100].

1661 Events resulting from the whole generation process are known as MC events.

1662 **3.3 CMS detector simulation.**

1663 After generation, MC events contain the physics of the collisions but they are not
 1664 ready to be compared to the events recorded by the experiment since these recorded
 1665 events correspond to the response of the detection systems to the interaction with
 1666 the particles traversing them. The simulation of the CMS detector has to be applied
 1667 on top of the event generation; it is simulated with a MC toolkit for the simulation
 1668 of particles passing through matter called Geant4 which is also able to simulate the
 1669 electronic signals that would be measured by all detectors inside CMS.

1670 The simulation takes the generated particles contained in the MC events as input,
 1671 makes them pass through the simulated geometry, and models physics processes that
 1672 particles experience during their passage through matter. The full set of results from
 1673 particle-matter interactions corresponds to the simulated hit which contains informa-
 1674 tion about the energy loss, momentum and position. Particles of the input event are
 1675 called *primary*, while the particles originating from GEANT4-modeled interactions of
 1676 a primary particle with matter are called a *secondary*. Simulated hits are the input
 1677 of subsequent modules that emulate the response of the detector readout system and

1678 triggers. The output from the emulated detection systems and triggers is known as
 1679 digitization [101, 102].

1680 The modeling of the CMS detector corresponds to the accurate modeling of the
 1681 interaction among particles, the detector material, and the magnetic field. This
 1682 simulation procedure includes the following standard steps

1683 • Modeling of the Interaction Region.

1684 • Modeling of the particle passage through the hierarchy of volumes that compose
 1685 CMS detector and of the accompanying physics processes.

1686 • Modeling of the effect of multiple interactions per beam crossing and/or the
 1687 effect of events overlay (Pile-Up simulation).

1688 • Modeling of the detector's electronics response, signal shape, noise, calibration
 1689 constants (digitization).

1690 In addition to the full simulation, i.e., a detailed detector simulation, a faster
 1691 simulation (FastSim) have been developed, that may be used where much larger
 1692 statistics are required. In FastSim, detector material effects are parametrized and
 1693 included in the hits; those hits are used as input of the same higher-level algorithms³
 1694 used to analyze the recorded events. In this way, comparisons between fast and full
 1695 simulations can be performed [104].

1696 After the full detector simulation, the output events can be directly compared
 1697 to events actually recorded in the CMS detector. The collection of MC events that
 1698 reproduces the expected physics for a given process is known as MC sample.

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

1699 **3.4 Event reconstruction.**

1700 The CMS experiment use the *particle-flow event reconstruction algorithm (PF)* to do
1701 the reconstruction of particles produced in pp collisions. Next sections will present
1702 a basic description of the *Elements* used by PF (tracker tracks, energy clusters, and
1703 muon tracks), based in the References [105, 106] where more detailed descriptions can
1704 be found.

1705 **3.4.1 Particle-Flow Algorithm.**

1706 Each of the several sub detection systems of the CMS detector is dedicated to identify
1707 an specific type of particles, i.e., photons and electrons are absorbed by the ECAL
1708 and their reconstruction is based on ECAL information; hadrons are reconstructed
1709 from clusters in the HCAL while muons are reconstructed from hits in the muon
1710 chambers. PF is designed to correlate signals from all the detector layers (tracks and
1711 energy clusters) in order to reconstruct and identify each final state particle and its
1712 properties as sketched in Figure 3.2.

1713 For instance, a charged hadron is identified by a geometrical connection, known
1714 as *link*, between one or more calorimeter clusters and a track in the tracker, provided
1715 there are no hits in the muon system; combining several measurements allows a better
1716 determination of the energy and charge sign of the charged hadron.

1717 **Charged-particle track reconstruction.**

1718 The strategy used by PF in order to reconstruct tracks is called *Iterative Tracking*
1719 which occurs in four steps

- 1720 • Seed generation where initial track candidates are found by looking for a combi-
1721 nation of hits in the pixel detector, strip tracker, and muon chambers. In total

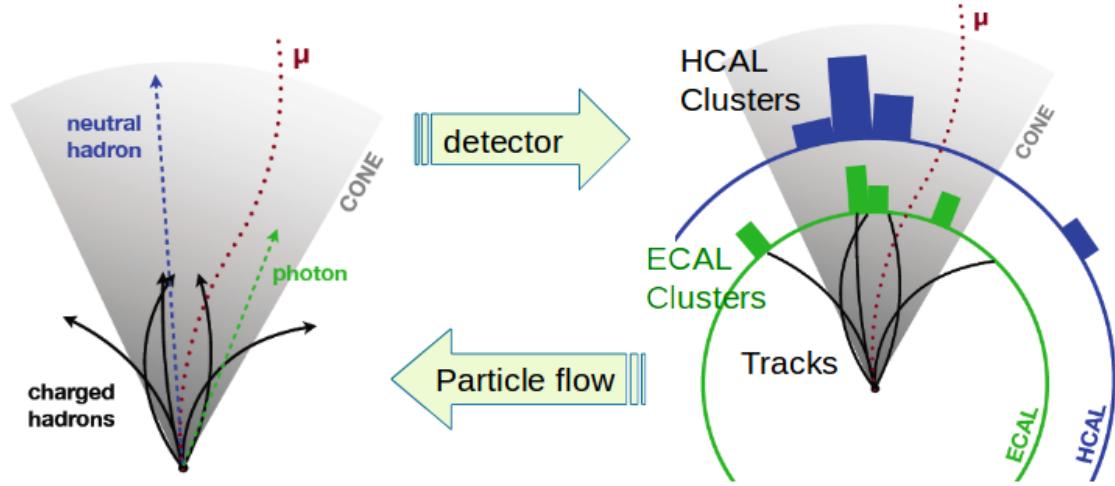


Figure 3.2: Particle flow algorithm. Information from the several CMS detection systems is provided as input to the algorithm which then combines it to identify and reconstruct all the particles in the final state and their properties. Reconstruction of simulated events is also performed by providing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

1722 ten iterations are performed, each one with a different seeding requirement.
 1723 Seeds are used to estimate the trajectory parameters and uncertainties at the
 1724 time of the full track reconstruction. Seeds are also considered track candidates.

- 1725 • Track finding using a tracking software known as Combinatorial Track Finder
 1726 (CTF) [108]. The seed trajectories are extrapolated along the expected flight
 1727 path of a charged particle, in agreement to the trajectory parameters obtained
 1728 in the first step, in an attempt to find additional hits that can be assigned to
 1729 the track candidates.

- 1730 • Track-fitting where the found tracks are passed as input to a module which
 1731 provides the best estimate of the parameters of each trajectory.

- 1732 • Track selection where track candidates are submitted to a selection which dis-
 1733 cards those that fail a set of defined quality criteria.

1734 Iterations differ in the seeding configuration and the final track selection as elab-

1735 orated in References [105, 106]. In the first iteration, high p_T tracks and tracks pro-
 1736 duced near to the interaction region are identified and those hits are masked thereby
 1737 reducing the combinatorial complexity. Next, iterations search for more complicated
 1738 tracks, like low p_T tracks and tracks from b hadron decays, which tend to be displaced
 1739 from the interaction region.

1740 **Vertex reconstruction.**

1741 During the track reconstruction, an extrapolation toward to the calorimeters is per-
 1742 formed in order to match energy deposits; that extrapolation is performed also toward
 1743 the beamline in order to find the origin of the track known as *vertex*. The vertex re-
 1744 construction is performed by selecting from the available reconstructed tracks, those
 1745 that are consistent with being originated in the interaction region where pp collisions
 1746 are produced. The selection involves a requirement on the number of tracker (pixel
 1747 and strip) hits and the goodness of the track fit.

1748 Selected tracks are clustered using a *deterministic annealing algorithm* (DA)⁴. A
 1749 set of candidate vertices and their associated tracks, resulting from the DA, are then
 1750 fitted with an *adaptive vertex fitter* (AVF) to produce the best estimate of the vertices
 1751 locations.

1752 The p_T of the tracks associated to a reconstructed vertex is added, squared and
 1753 used to organize the vertices; the vertex with the highest squared sum is designated
 1754 as the *primary vertex* (*PV*) while the rest are designated as PU vertices.

1755 **Calorimeter clustering.**

1756 After traversing the CMS tracker system, electrons, photons and hadrons deposit their
 1757 energy in the ECAL and HCAL cells. The PF clustering algorithm aims to provide

⁴ DA algorithm and AVF are described in detail in References [110, 111]

1758 a high detection efficiency even for low-energy particles and an efficient distinction
 1759 between close energy deposits. The clustering runs independently in the ECAL barrel
 1760 and endcaps, HCAL barrel and endcaps, and the two preshower layers, following two
 1761 steps

- 1762 • cells with an energy larger than a given seed threshold and larger than the energy
 1763 of the neighboring cells are identified as cluster seeds. The neighbor cells are
 1764 those that either share a side with the cluster seed candidate, or the eight closest
 1765 cells including cells that only share a corner with the seed candidate.
- 1766 • cells with at least a corner in common with a cell already in the cluster seed
 1767 and with an energy above a cell threshold are grouped into topological clusters.

1768 Clusters formed in this way are known as *particle-flow clusters*. With this cluster-
 1769 ing strategy, it is possible to detect and measure the energy and direction of photons
 1770 and neutral hadrons as well as differentiate these neutral particles from the charged
 1771 hadron energy deposits. In cases involving charged hadrons for which the track pa-
 1772 rameters are not determined accurately, for instance, low-quality and high- p_T tracks,
 1773 clustering helps in the energy measurements.

1774 **Electron track reconstruction.**

1775 Although the charged-particle track reconstruction described above works for elec-
 1776 trons, they lose a significant fraction of their energy via bremsstrahlung photon radi-
 1777 ation before reaching the ECAL; thus, the reconstruction performance depends on the
 1778 ability to measure also the radiated energy. The reconstruction strategy, in this case,
 1779 requires information from the tracking system and from the ECAL. Bremsstrahlung
 1780 photons are emitted at similar η values to that of the electron but at different values
 1781 of ϕ ; therefore, the radiated energy can be recovered by grouping ECAL clusters in a

1782 η window over a range of ϕ around the electron direction. The group is called ECAL
 1783 supercluster.

1784 Electron candidates from the track-seeding and ECAL super clustering are merged
 1785 into a single collection which is submitted to a full electron tracking fit with a
 1786 Gaussian-sum filter (GSF) [109]. The electron track and its associated ECAL su-
 1787 percluster form a *particle-flow electron*.

1788 **Muon track reconstruction.**

1789 Given that the CMS detector is equipped with a muon spectrometer capable to iden-
 1790 tify and measure the momentum of the muons traversing it, the muon reconstruction
 1791 is not specific to PF; therefore, three different muon types are defined

- 1792 • *Standalone muon.* A clustering on the DTs or CSCs hits is performed to form
 1793 track segments; those segments are used as seeds for the reconstruction in the
 1794 muon spectrometer. All DTs, CSCs, and RPCs hits along the muon trajectory
 1795 are combined and fitted to form the full track. The fitting output is called a
 1796 *standalone-muon track*.
- 1797 • *Tracker muon.* Each track in the inner tracker with p_T larger than 0.5 GeV and
 1798 a total momentum p larger than 2.5 GeV is extrapolated to the muon system.
 1799 A *tracker muon track* corresponds to a extrapolated track that matches at least
 1800 one muon segment.
- 1801 • *Global muon.* When tracks in the inner tracker (inner tracks) and standalone-
 1802 muon tracks are matched and turn out being compatibles, their hits are com-
 1803 bined and fitted to form a *global-muon track*.

1804 Global muons sharing the same inner track with tracker muons are merged into
 1805 a single candidate. PF muon identification uses the muon energy deposits in ECAL,
 1806 HCAL, and HO associated with the muon track to improve the muon identification.

1807 **Particle identification and reconstruction.**

1808 PF elements are connected by a linker algorithm that tests the connection between any
 1809 pair of elements; if they are found to be linked, a geometrical distance that quantifies
 1810 the quality of the link is assigned. Two elements may be linked indirectly through
 1811 common elements. Linked elements form *PF blocks* and each PF block may contain
 1812 elements originating in one or more particles. Links can be established between
 1813 tracks, between calorimeter clusters, and between tracks and calorimeter clusters.
 1814 The identification and reconstruction start with a PF block and proceed as follows

1815 • Muons. An *isolated global muon* is identified by evaluating the presence of
 1816 inner track and energy deposits close to the global muon track in the (η, ϕ)
 1817 plane, i.e., in a particular point of the global muon track, inner tracks and
 1818 energy deposits are sought within a radius of $\Delta R = 0.3$ (see eqn. 2.7) from the
 1819 muon track; if they exist and the p_T of the found track added to the E_T of the
 1820 found energy deposit does not exceed 10% of the muon p_T then the global muon
 1821 is an isolated global muon. This isolation condition is stringent enough to reject
 1822 hadrons misidentified as muons.

1823 *Non-isolated global muons* are identified using additional selection requirements
 1824 on the number of track segments in the muon system and energy deposits along
 1825 the muon track. Muons inside jets are identified with more stringent criteria
 1826 in isolation and momentum as described in Reference [112]. The PF elements
 1827 associated with an identified muon are masked from the PF block.

- 1828 ● Electrons are identified and reconstructed as described above plus some addi-
 1829 tional requirements on fourteen variables like the amount of energy radiated,
 1830 the distance between the extrapolated track position at the ECAL and the po-
 1831 sition of the associated ECAL supercluster, among others, which are combined
 1832 in an specialized multivariate analysis strategy that improves the electron iden-
 1833 tification. Tracks and clusters used to identify and reconstruct electrons are
 1834 masked in the PF block.
- 1835 ● Isolated photons are identified from ECAL superclusters with E_T larger than 10
 1836 GeV, for which the energy deposited at a distance of 0.15, from the supercluster
 1837 position on the (η, ϕ) plane, does not exceed 10% of the supercluster energy;
 1838 note that this is an isolation requirement. In addition, there must not be links
 1839 to tracks. Clusters involved in the identification and reconstruction are masked
 1840 in the PF block.
- 1841 ● Bremsstrahlung photons and prompt photons tend to convert to electron-positron
 1842 pairs inside the tracker, therefore, a dedicated finder algorithm is used to link
 1843 tracks that seem to originate from a photon conversion; in case those two tracks
 1844 are compatible with the direction of a bremsstrahlung photon, they are also
 1845 linked to the original electron track. Photon conversion tracks are also masked
 1846 in the PF block.
- 1847 ● The remaining elements in the PF block are used to identify hadrons. In the
 1848 region $|\eta| \leq 2.5$, neutral hadrons are identified with HCAL clusters not linked
 1849 to any track while photons from neutral pion decays are identified with ECAL
 1850 clusters without links to tracks. In the region $|\eta| > 2.5$ ECAL clusters linked to
 1851 HCAL clusters are identified with a charged or neutral hadron shower; ECAL
 1852 clusters with no links are identified with photons. HCAL clusters not used yet,

1853 are linked to one or more unlinked tracks and to an unlinked ECAL in order to
 1854 reconstruct charged-hadrons or a combination of photons and neutral hadrons
 1855 according to certain conditions on the calibrated calorimetric energy.

- 1856 • Charged-particle tracks may be liked together when they converge to a *sec-*
 1857 *ondary vertex (SV)* displaced from the IP where the PV and PU vertices are
 1858 reconstructed; at least three tracks are needed in that case, of which at most
 1859 one has to be an incoming track with hits in tracker region between a PV and
 1860 the SV.

1861 The linker algorithm, as well as the whole PF algorithm, has been validated and
 1862 commissioned; results from that validation are presented in the Reference [105].

1863 **Jet reconstruction.**

1864 Quarks and gluons may be produced in the pp collisions, therefore, their hadronization
 1865 will be seen in the detector as a shower of hadrons and their decay products in the
 1866 form of a *jet*. Two classes of clustering algorithms have been developed based in
 1867 their jet definition [113]:

- 1868 • Iterative cone algorithms (IC). Jets are defined in terms of circles of fixed radius
 1869 R in the $\eta\text{-}\phi$ plane, known as *stable cones*, for which the sum of the momenta
 1870 of all the particles within the cone points in the same direction as the center
 1871 of the circle. The seed of the iteration is the hardest non-isolated particle in
 1872 the event, then, the resulting momentum direction is assigned as the new cone
 1873 direction and a new iteration starts; iteration process stops when the cone if
 1874 found to be stable.

1875 • Sequential recombination algorithms. The distance between non-isolated par-
 1876 ticles is calculated; if that distance is below a threshold, these particles are
 1877 recombined into a new object. The sequence is repeated until the separation
 1878 between the recombined object and any other particle is above certain thresh-
 1879 old; the recombined object is called a jet and the algorithm starts again with
 1880 the remaining particles.

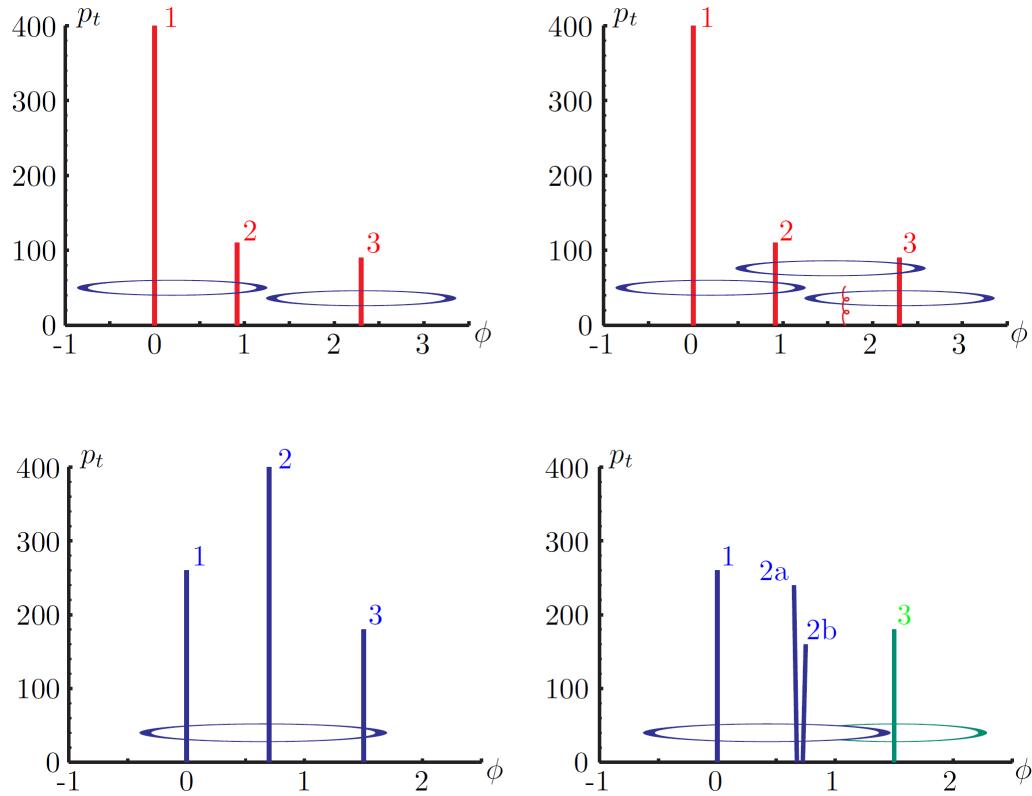


Figure 3.3: Stable cones identification using IC algorithms [113].

1881 Two conditions are of particular importance for the clustering algorithms, *infrared*
 1882 and *collinear (IRC) safety*. In order to explain the concept of infrared (IR) safety,
 1883 consider an event with three hard particles as shown in the top left side of Figure 3.3,
 1884 two stable cones are found and then two jets are identified; if a soft gluon is added, as
 1885 shown in the top right side of Figure 3.3, three stable cones are found and the three

1886 hard particles are now clustered into a single jet. If the addition of soft particles
 1887 change the outcome of the clustering, then it is said that the algorithm is IR unsafe.
 1888 Soft radiation is highly likely in perturbative QCD, which dominates the physics of
 1889 the jets, and then IR unsafe effect leads to divergences [113].

1890 The concept of collinear safety can also be explained considering a three hard
 1891 particles event, as shown in the bottom left side of Figure 3.3, where one stable cone
 1892 containing all three particles is found and one jet is identified; if the hardest particle
 1893 is split into two collinear particles (2a and 2b) in the bottom right side of Figure 3.3,
 1894 then the clustering results in a different jet identification and the algorithm is said
 1895 to be collinear unsafe. The collinear unsafe effect leads to divergences in jet cross
 1896 section calculations [114].

1897 It has been determined that IC algorithms are IRC unsafe, and therefore, they
 1898 have to be replaced by algorithms that not only provide the finite perturbative results
 1899 from theoretical computations, but also that are not highly dependent on underlying
 1900 event and pileup effects which leads to significant corrections [113].

1901 The sequential recombination algorithms arise as the IRC safe alternative used by
 1902 the CMS experiment; in particular the anti- k_t algorithm which is a generalization of
 1903 the previously existing k_t [115] and Cambridge/Aachen [116] jet clustering algorithms.

1904 The anti- k_t algorithm is used to perform the jet reconstruction by clustering those
 1905 PF particles within a cone (see Figure 3.4); previously, isolated electrons, isolated
 1906 muons, and charged particles associated with other interaction vertices are excluded
 1907 from the clustering.

1908 The anti- k_t algorithm proceeds in a sequential recombination of PF particles; the
 1909 distance between particles i and j (d_{ij}) and the distance between particles and the
 1910 beam are defined as

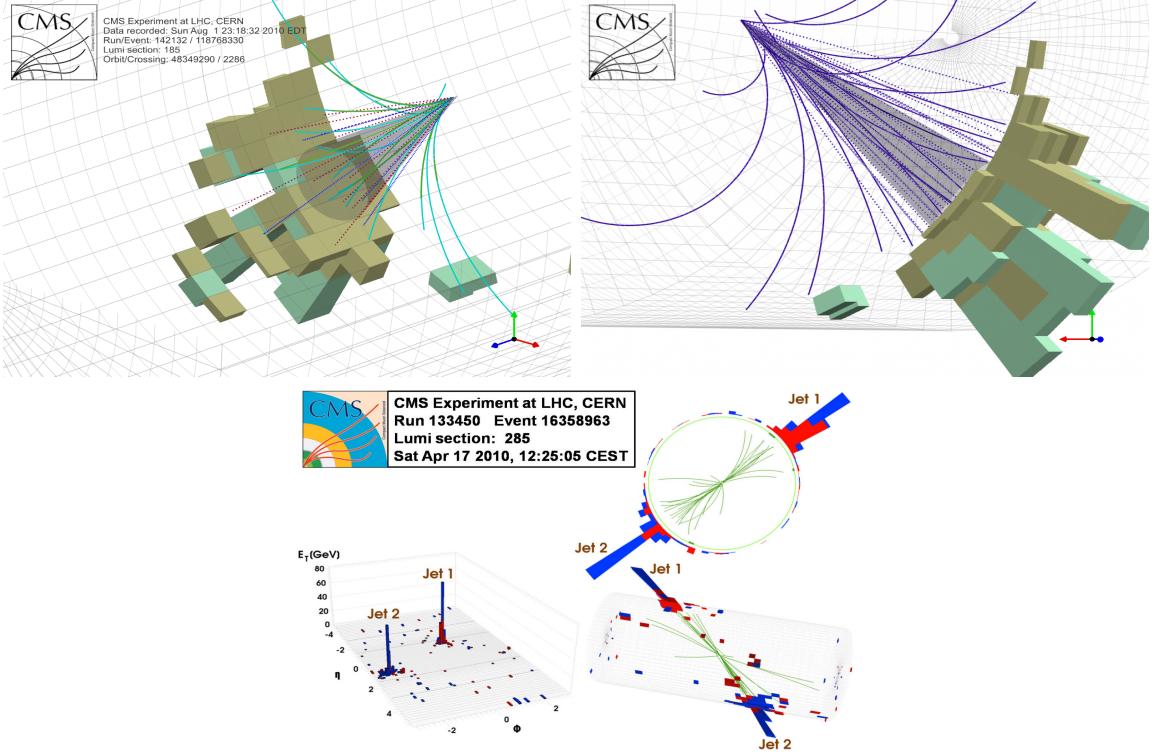


Figure 3.4: Jet reconstruction performed by the anti- k_t algorithm. Top: Two different views of a CMS recorded event are presented. Continuous lines correspond to tracks left by charged particles in the tracker while dotted lines are the imaginary paths followed by neutral particles. The green cubes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

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

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

1911 where $\Delta_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$, k_{ti} , y_i and ϕ_i are the transverse momentum, 1912 rapidity and azimuth of particle i respectively and R is the called jet radius. For all 1913 the remaining PF particles, after removing the isolated ones, d_{ij} and d_{iB} are calcu-

1914 lated⁵ and the smallest is identified; if it is a d_{ij} , particles i and j are replaced with
 1915 a new object whose momentum is the vectorial sum of the combined particles. If the
 1916 smallest distance is a d_{iB} the clustering process ends, the object i (which at this stage
 1917 should be a combination of several PF particles) is declared as a *Particle-flow-jet* (PF
 1918 jet) and all the associated PF particles are removed from the detector. The clustering
 1919 process is repeated until no PF particles remain. R is a free parameter that can be
 1920 adjusted according to the specific analysis conditions; usually, two values are used,
 1921 $R=0.4$ and $R=0.5$, giving the name to the so-called AK4-jet and AK5-jet respectively.

1922 An advantage of the anti- k_t algorithm over other clustering algorithms is the reg-
 1923 ularity of the boundaries of the resulting jets. For all known IRC safe algorithms,
 1924 soft radiation can introduce irregularities in the boundaries of the final jets; however,
 1925 anti- k_t algorithm is soft-resilient, meaning that jets shape is not affected by soft radi-
 1926 ation, which is a valuable property considering that knowing the typical shape of jets
 1927 makes experimental calibration of jets more simple. In addition, that soft-resilience
 1928 is expected to simplify certain theoretical calculations and reduce the momentum-
 1929 resolution loss caused by underlying-event (UE) and pileup contamination [114].

1930 The effect of the UE and pileup contamination over a jet identification, can be
 1931 seen as if soft events are added to the jet; for instance, if a soft event representing UE
 1932 or pileup is added to an event for which a set of jets J have been identified, and the
 1933 clustering is rerun on that new extended event, the outcome will be different in two
 1934 aspects: jets will contain some additional soft energy and the distribution of particles
 1935 in jets may have change; that effect is called *back-reaction*. The back-reaction effect in
 1936 the anti- k_t algorithm is suppressed not by the amount of momentum added to the jet
 1937 but by the jet transverse momentum $p_{T,J}$, which means that this strong suppression
 1938 leads to a smaller correction due to EU and pileup effect [114].

⁵ Notice that this is a combinatorial calculation.

1939 **Jet energy Corrections**

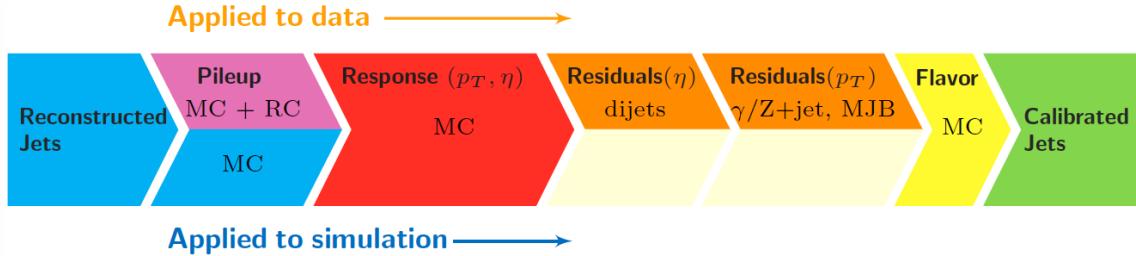


Figure 3.5: Jet energy correction diagram. Correction levels are applied sequentially in the indicated fixed order [120].

1940 Even though jets can be reconstructed efficiently, there are some effects that are
 1941 not included in the reconstruction and that lead to discrepancies between the re-
 1942 constructed results and the predicted results; in order to overcome these discrep-
 1943 ancies, a factorized model has been designed in the form of jet energy corrections
 1944 (JEC) [119, 120] applied sequentially as shown in the diagram of Figure 3.5.

1945 At each level, the jet four-momentum is multiplied by a scaling factor based on
 1946 jet properties, i.e., η , flavor, etc.

1947 • Level 1 correction removes the energy coming from pile-up. The scale factor is
 1948 determined using a MC sample of QCD dijet (2 jets) events with and without
 1949 pileup overlay; it is parametrized in terms of the offset energy density ρ , jet
 1950 area A , jet η and jet p_T . Different corrections are applied to data and MC due
 1951 to the detector simulation.

1952 • MC-truth correction accounts for differences between the reconstructed jet en-
 1953 ergy and the MC particle-level energy. The correction is determined on a QCD
 1954 dijet MC sample and is parametrized in terms of the jet p_T and η .

1955 • Residuals correct remaining small differences within jet response in data and
 1956 MC. The Residuals η -dependent correction compares jets of similar p_T in the

1957 barrel reference region. The Residuals p_T -dependent correct the jet absolute
 1958 scale (JES vs p_T).

- 1959 • Jet-flavor corrections are derived in the same way as MC-truth corrections but
 1960 using QCD pure flavor samples.

1961 ***b*-tagging of jets.**

1962 A particular feature of the hadrons containing bottom quarks (*b*-hadrons) is that
 1963 their lifetime is long enough to travel some distance before decaying, but it is not as
 1964 long as those of light quark hadrons; therefore, when looking at the hadrons produced
 1965 in pp collisions, *b*-hadrons decay typically inside the tracker rather than reaching the
 1966 calorimeters as some light-hadrons do. As a result, a *b*-hadron decay gives rise to a
 1967 displaced vertex (secondary vertex) with respect to the primary vertex as shown in
 1968 Figure 3.6; the SV displacement is in the order of a few millimeters. A jet resulting
 1969 from the decay of a *b*-hadron is called *b* jet; other jets are called light jets.

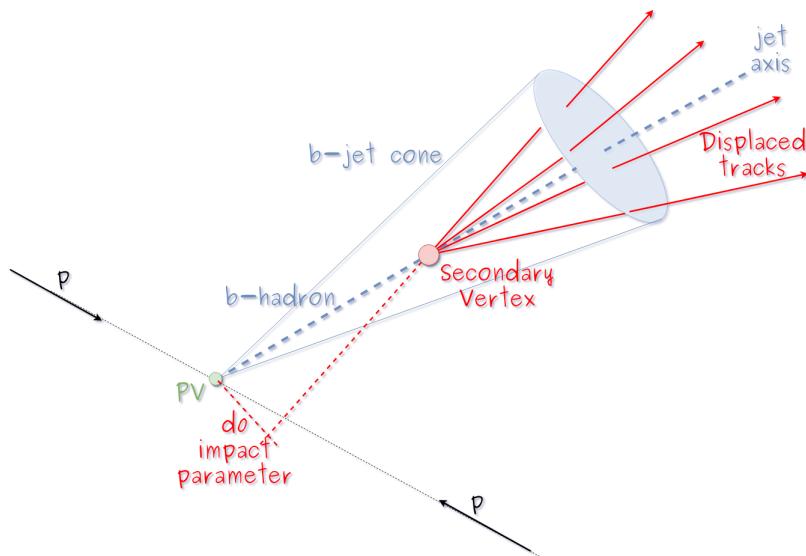


Figure 3.6: Secondary vertex in a *b*-hadron decay.

1970 Several methods to identify *b*-jets (*b*-tagging) have been developed; the method

1971 used in this thesis is known as *Combined Secondary Vertex* algorithm in its second
 1972 version (CSVv2) [121]. By using information of the impact parameter, the recon-
 1973 structed secondary vertices, and the jet kinematics as input in a multivariate analysis
 1974 that combines the discrimination power of each variable in one global discrimina-
 1975 tor variable, three working points (references): loose, medium and tight, are defined
 1976 which quantify the probabilities of mistag jets from light quarks as jets from b quarks;
 1977 10, 1 and 0.1 % respectively. Although the mistagging probability decreases with the
 1978 working point strength, the efficiency to correctly tag b -jets also decreases as 83, 69
 1979 and 49 % for the respective working point; therefore, a balance needs to be achieved
 1980 according to the specific requirements of the analysis.

1981 **Missing transverse energy.**

1982 The fact that proton bunches carry momentum along the z -axis implies that for
 1983 each event it is expected that the momentum in the transverse plane is balanced.
 1984 Imbalances are quantified by the missing transverse energy (MET) and are attributed
 1985 to several sources including particles escaping undetected through the beam pipe,
 1986 neutrinos produced in weak interactions processes which do not interact with the
 1987 detector and thus escaping without leaving a sign, or even undiscovered particles
 1988 predicted by models beyond the SM.

1989 The PF algorithm assigns the negative sum of the momenta of all reconstructed
 1990 PF particles to the *particle-flow MET* according to

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

1991 JEC are propagated to the calculation of the \vec{E}_T as described in the Reference [122].

1992 3.4.2 Event reconstruction examples

1993 Figures 3.7-3.9 show the results of the reconstruction performed on 3 recorded events.

1994 Descriptions are taken directly from the source.

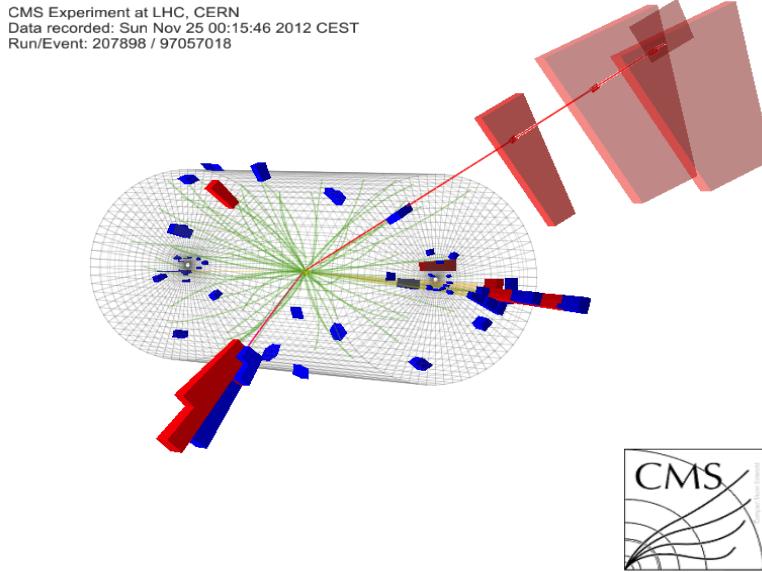


Figure 3.7: HIG-13-004 Event 1 reconstruction results; “HIG-13-004 Event 1: Event recorded with the CMS detector in 2012 at a proton-proton center-of-mass energy of 8 TeV. The event shows characteristics expected from the decay of the SM Higgs boson to a pair of τ leptons. Such an event is characterized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

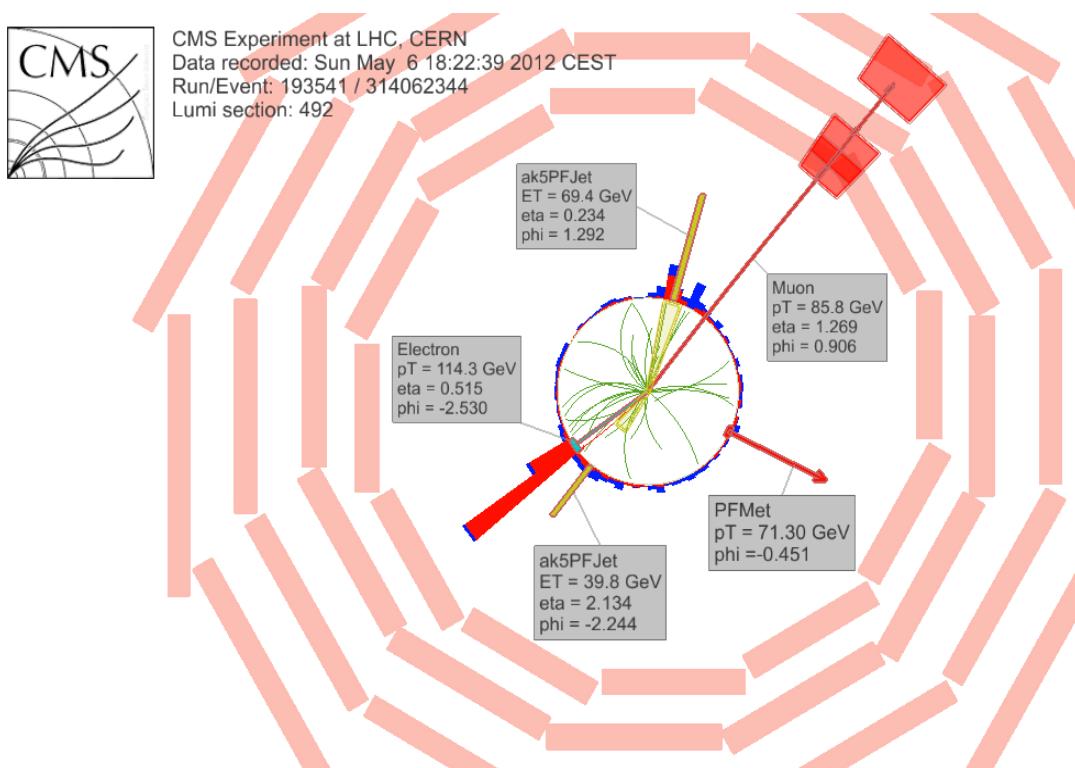


Figure 3.8: $e\mu$ event reconstruction results; “An $e\mu$ event candidate selected in 8 TeV data, as seen from the direction of the proton beams. The kinematics of the main objects used in the event selection are highlighted: two isolated leptons and two particle-flow jets. The reconstructed missing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

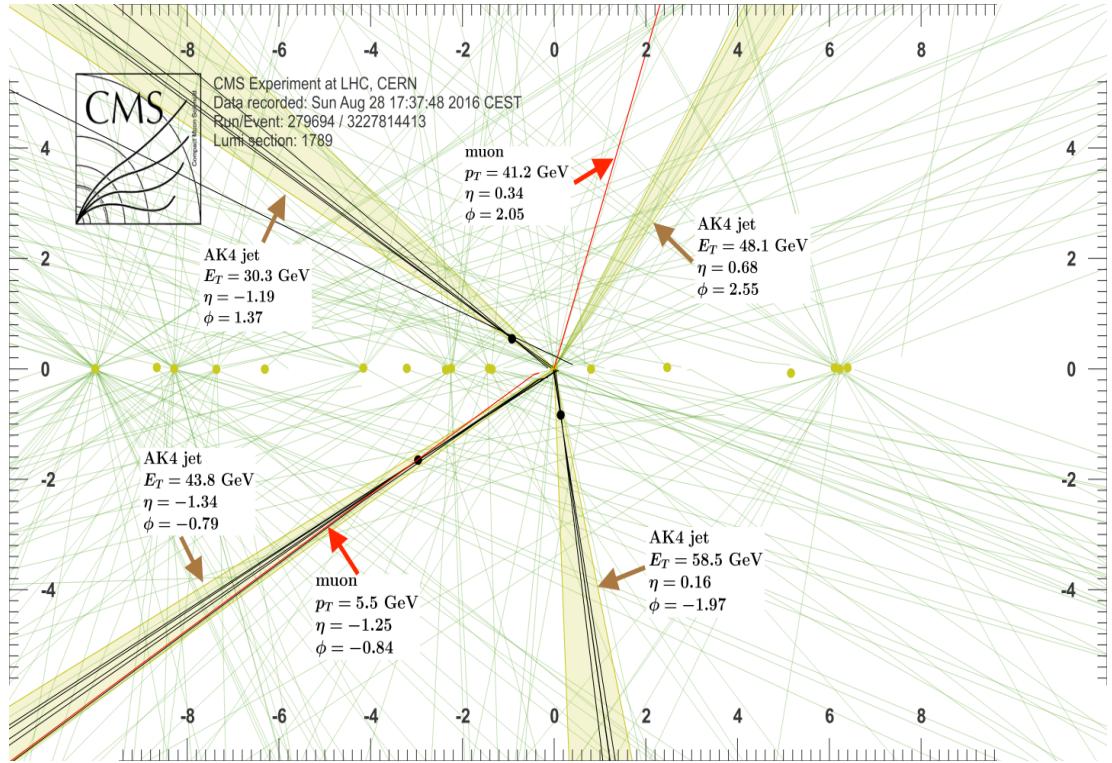


Figure 3.9: Recorded event reconstruction results; “Recorded event (ρ - z projection) with three jets with $p_T > 30$ GeV with one displaced muon track in 2016 data collected at 13 TeV. Each of the three jets has a displaced reconstructed vertex. The jet with $p_T(j) = 43.8$ GeV, $\eta(j) = -1.34$, $\phi(j) = -0.79$ 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].

₁₉₉₅ **Chapter 5**

₁₉₉₆ **Statistical methods**

₁₉₉₇ In the course of analyzing the data sets provided by the CMS experiment and used in
₁₉₉₈ this thesis, several statistical tools have been employed; in this chapter, a description
₁₉₉₉ of these tools will be presented, starting with the general statement of the multivariate
₂₀₀₀ analysis methods, followed by the particularities of the Boosted Decision Trees (BDT)
₂₀₀₁ method and its application to the classification problem. Statistical inference methods
₂₀₀₂ used will also be presented. This chapter is based mainly on References [126–128].

₂₀₀₃ **5.1 Multivariate analysis**

₂₀₀₄ Multivariate data analysis (MVA) makes use of the statistical techniques developed to
₂₀₀₅ analyze more than one variable at once, taking into account all the correlations among
₂₀₀₆ variables. MVA is employed in a variety of fields like consumer and market research,
₂₀₀₇ quality control and process optimization. Using MVA it is possible to identify the
₂₀₀₈ dominant patterns in a data sample, like groups, outliers and trends, and determine
₂₀₀₉ to which group a set of values belong; in the particle physics context, MVA methods
₂₀₁₀ are used to perform the selection of certain type of events from a large data set.

2011 Processes with small cross section, such as the tHq process ($\sigma_{SM}(\sqrt{s} = 13\text{TeV}) =$
 2012 70.96 fb), are hard to detect in the presence of the processes with larger cross sections,
 2013 $\sigma_{SM}^{t\bar{t}}(\sqrt{s} = 13\text{TeV}) = 823.44$ fb for instance; therefore, only a small fraction of the data
 2014 contains events of interest (signal), the major part is signal-like events, which mimic
 2015 signal characteristics but belong to different processes, so they are a background to
 2016 the process of interest. This implies that it is not possible to say with certainty
 2017 that a given event is a signal or a background and statistical methods should be
 2018 involved. In that sense, the challenge can be formulated as one where a set of events
 2019 have to be classified according to certain special features; these features correspond
 2020 to the measurements of several parameters like energy or momentum, organized in a
 2021 set of *input variables*. The measurements for each event can be written in a vector
 2022 $\mathbf{x} = (x_1, \dots, x_n)$ for which

- 2023 • $f(\mathbf{x}|s)$ is the probability density (*likelihood function*) that \mathbf{x} is the set of mea-
 2024 sured values given that the event is a signal event (signal hypothesis).
- 2025 • $f(\mathbf{x}|b)$ is the probability density (*likelihood function*) that \mathbf{x} is the set of mea-
 2026 sured values given that the event is a background event (background hypothe-
 2027 sis).

2028 Figure 5.1 shows three ways to perform a classification of events for which mea-
 2029 surements of two properties, i.e., two input variables x_1 and x_2 , have been performed;
 2030 blue circles represent signal events while red triangles represent background events.
 2031 The classification on the left is *cut-based* requiring $x_1 < c_1$ and $x_2 < c_2$; usually the
 2032 cut values (c_1 and c_2) are chosen according to some knowledge about the event pro-
 2033 cess. In the middle plot, the classification is performed using a linear function of
 2034 the input variables, hence the boundary is a straight line, while in the right plot the

2035 the relationship between input variables is not linear thus the boundary is not linear
 2036 either.

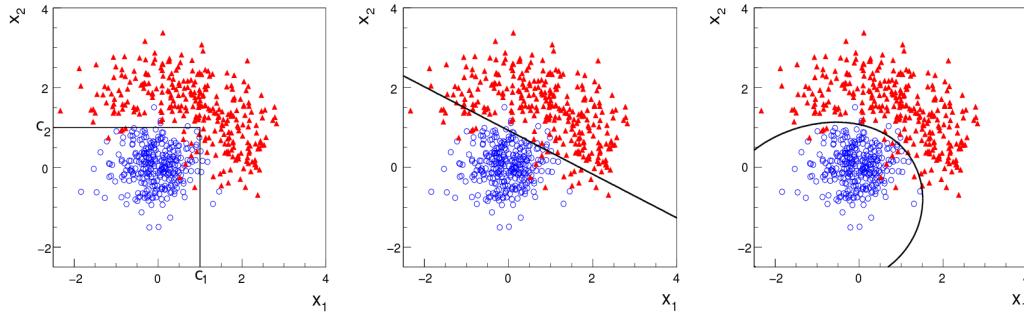


Figure 5.1: Scatter plots-MVA event classification. Distribution of two input variables x_1 and x_2 measured for a set of events; blue circles represent signal events and red triangles represent background events. The classification is based on cuts (left), linear boundary (center), and nonlinear boundary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

2037 In general, the boundary can be parametrized in terms of the input variables such
 2038 that the cut is set on the parametrization instead of on the variables, i.e., $y(\mathbf{x}) = y_{cut}$
 2039 with y_{cut} being a constant; thus, the acceptance or rejection of an event is based on
 2040 which side of the boundary the event is located. If $y(\mathbf{x})$, usually called *test statistic*,
 2041 has functional form, it can be used to determine the probability distribution functions
 2042 $p(y|s)$ and $p(y|b)$ and then perform a test statistic with a single cut on the scalar
 2043 variable y .

2044 Figure 5.2 shows an example of what would be the probability distribution func-
 2045 tions under the signal and background hypotheses for a scalar test statistic with a cut
 2046 on the classifier y . Note that the tails of the distributions indicate that some signal
 2047 events fall in the rejection region and some background events fall on the acceptance
 2048 region; therefore, it is convenient to define the *efficiency* with which events of a given
 2049 type are accepted. The signal and background efficiencies are given by

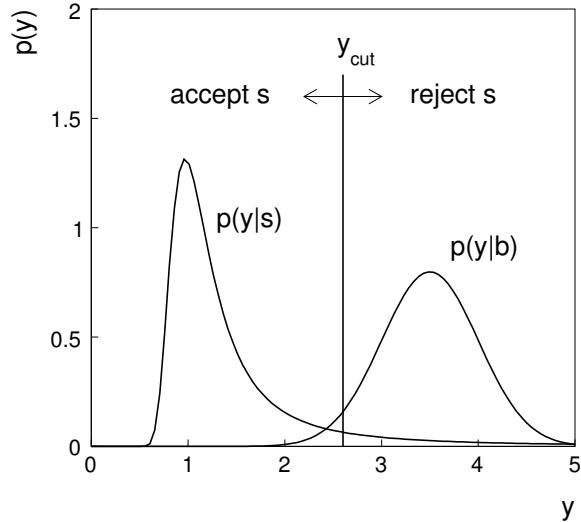


Figure 5.2: Distributions of the scalar test statistic $y(\mathbf{x})$ under the signal and background hypotheses. [126]

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

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

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

¹ β is the fraction of signal events that fall out of the acceptance region

2058 **5.1.1 Decision trees**

2059 For this thesis, the implementation of the MVA strategy, described above, is per-
 2060 formed through decision trees by using the TMVA software package [127] included
 2061 in the ROOT analysis framework [129]. In a simple picture, a decision tree classifies
 2062 events according to their input variables values by setting a cut on each input variable
 2063 and checking which events are on which side of the cut, just as proposed in the MVA
 2064 strategy, but in addition, as a machine learning algorithm, decision trees offer the
 2065 possibility to be trained and then perform the classification efficiently.

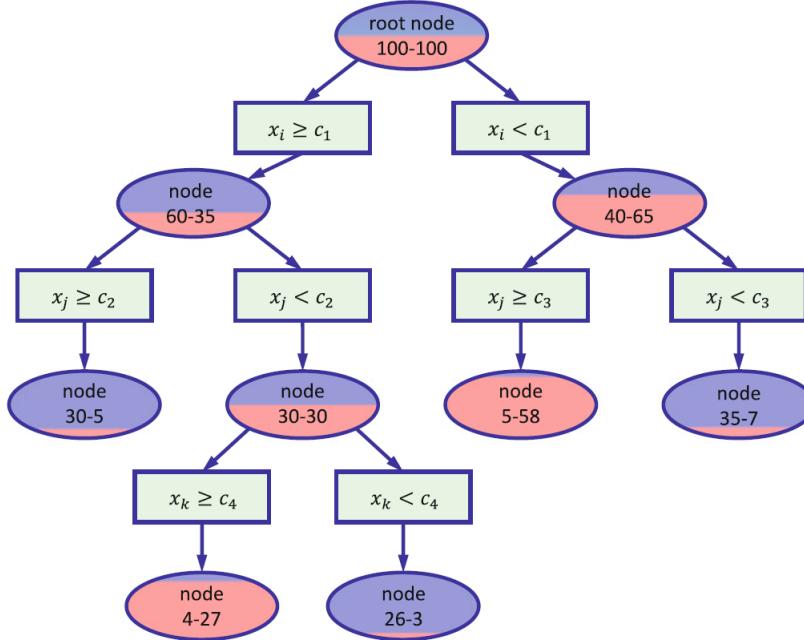


Figure 5.3: Example of a decision tree. Each node is fed with a MC sample mixing signal and background events (left-right numbers); nodes colors represent the relative number of signal/background events [128].

2066 The training or growing of a decision tree is the process where the rules for clas-
 2067 sifying events are defined; this process is represented in Figure 5.3 and consists of
 2068 several steps:

- 2069 • take MC samples of signal and background events and split them into two parts

2070 each; the first parts will be used in the decision tree training, while the second
 2071 parts will be used for testing the final classifier obtained from the training.
 2072 Each event has associated a set of input variables $\mathbf{x} = (x_1, \dots, x_n)$ which serve
 2073 to distinguish between signal and background events. The training sample is
 2074 taken in at the *root node*.

- 2075 • Pick one variable, say x_i .
- 2076 • Pick one value of x_i , each event has its own value of x_i , and split the training
 2077 sample into two subsamples B_1 and B_2 ; B_1 contains events for which $x_i < c_1$
 2078 while B_2 contains the rest of the training events;
- 2079 • scan all possible values of x_i and find the splitting value that provides the *best*
 2080 classification², i.e., B_1 is mostly made of signal events while B_2 is mostly made
 2081 of background events.
- 2082 • It is possible that variables other than the picked one produce a better classi-
 2083 fication, hence, all the variables have to be evaluated. Pick the next variable,
 2084 say x_j , and repeat the scan over its possible values.
- 2085 • At the end, all the variables and their values will have been scanned, the *best*
 2086 variable and splitting value will have been identified, say x_1, c_1 , and there will
 2087 be two nodes fed with the subsamples B_1 and B_2 .

2088 Nodes are further split by repeating the decision process until a given number of
 2089 final nodes is obtained, nodes are largely dominated by either signal or background
 2090 events, or nodes have too few events to continue. Final nodes are called *leaves* and
 2091 they are classified as signal or background leaves according to the class of the majority
 2092 of events in them. Each *branch* in the tree corresponds to a sequence of cuts.

² Quality of the classification will be treated in the next paragraph.

2093 The quality of the classification at each node is evaluated through a separation
 2094 criteria; there are several of them but the *Gini Index* (G) is the one used in the
 2095 decision trees trained for the analysis in this thesis. G is written in terms of the
 2096 purity (P), i.e., the fraction of signal events in the samples after the separation is
 2097 made; it is given by

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

2098 note that $P=0.5$ at the root node while $G=0$ for pure leaves. For a node A split into
 2099 two nodes B_1 and B_2 the G gain is

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

2100 The *best* classification corresponds to that for which the gain of G is maximized;
 2101 hence, the scanning over all the variables in an event and their values is of great
 2102 importance.

2103 In order to provide a numerical output for the classification, events in a sig-
 2104 nal(background) leaf are assigned a score of 1(-1) each, defining in this way the
 2105 decision tree *classifier/weak learner* as

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

2106 Figure 5.4 shows an example of the classification of a sample of events, containing
 2107 two variables, performed by a decision tree.

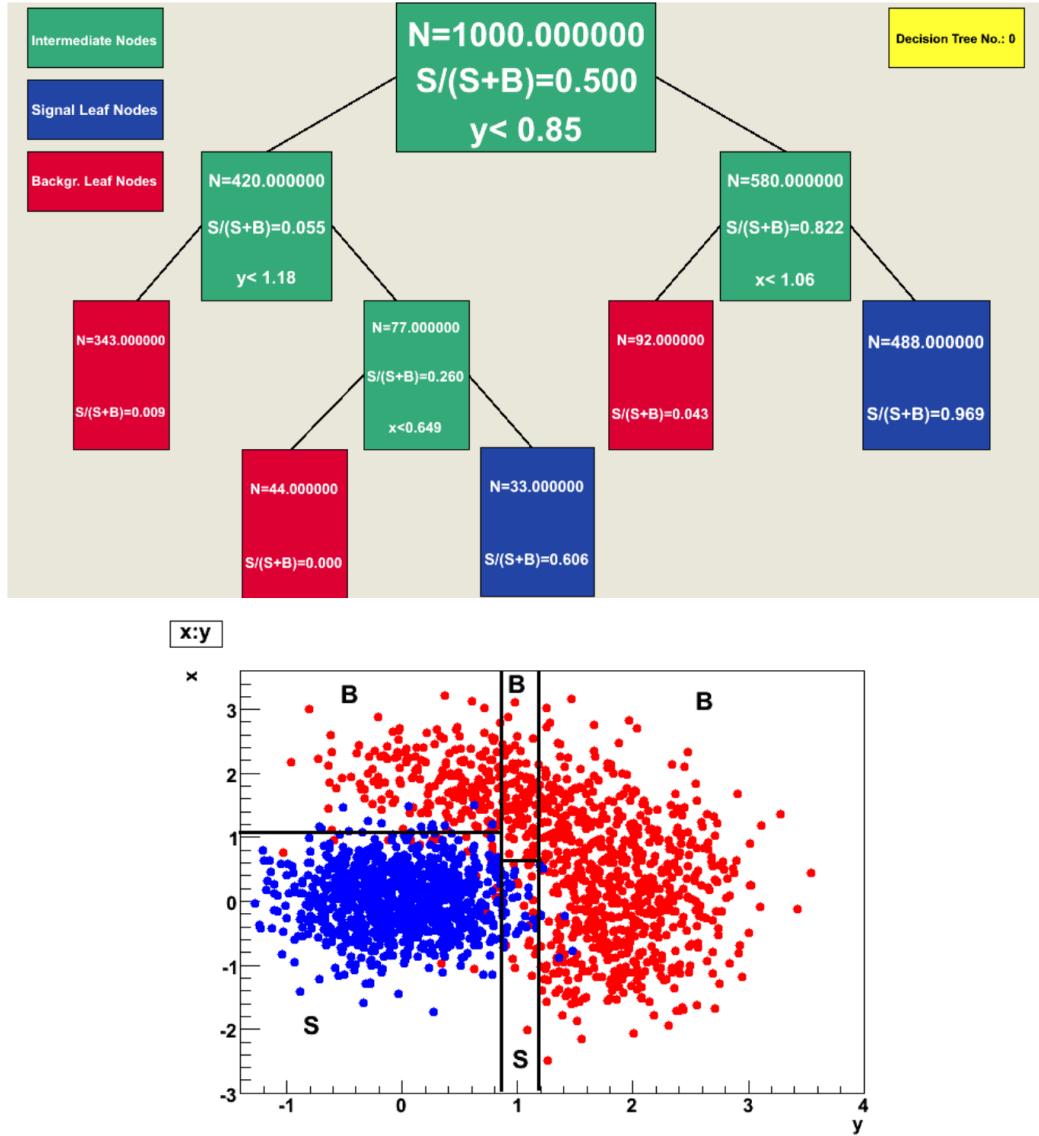


Figure 5.4: Example of a decision tree output. Each leaf, blue for signal events and red for background events, is represented by a region in the variables phase space [130].

2108 5.1.2 Boosted decision trees (BDT).

2109 Event misclassification occurs when a training event ends up in the wrong leaf, i.e., a
 2110 signal event ends up in a background leaf or a background event ends up in a signal
 2111 leaf. A way to correct it is to assign a weight to the misclassified events and train
 2112 a second tree using the reweighted events; the event reweighting is performed by a

2113 boosting algorithm in such a way that when used in the training of a new decision
 2114 tree the *boosted events* get correctly classified. The process is repeated iteratively
 2115 adding a new tree to the forest and creating a set of classifiers, which are combined
 2116 to create the next classifier; the final classifier offers more stability³ and has a smaller
 2117 misclassification rate than any individual ones. The resulting tree collection is known
 2118 as a *boosted decision tree (BDT)*.

2119 Thus, purity of the sample is generalized to

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

2120 where w_s and w_b are the weights of the signal and background events respectively;
 2121 the Gini index is also generalized

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

2122 with n the number of events in the node. The final score of an event, after pass-
 2123 ing through the forest, is calculated as the renormalized sum of all the individual
 2124 (possibly weighted) scores; thus, high(low) score implies that the event is most likely
 2125 signal(background).

2126 The boosting procedure, implemented in the *Gradient boosting* algorithm used in
 2127 this thesis, produces a classifier $F(\mathbf{x})$ which is the weighted sum of the individual
 2128 classifiers obtained after each iteration, i.e.,

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

2129 where M is the number of trees in the forest. The *loss function* $L(F, y)$ represents the

³ 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.

2130 deviation between the classifier $F(\mathbf{x})$ response and the true value y obtained from the
 2131 training sample (1 for signal events and -1 for background event), according to

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

2132 thus, the reweighting is employed to ensure the minimization of the loss function; a
 2133 more detailed description of the minimization procedure can be found in Reference
 2134 [131]. The final classifier output is later used as a final discrimination variable, labeled
 2135 as *BDT output/response*.

2136 5.1.3 Overtraining

2137 Decision trees offer the possibility to have as many nodes as desired in order to
 2138 reduce the misclassification to zero (in theory); however, when a classifier is too much
 2139 adjusted to a particular training sample, the classifier's response to a slightly different
 2140 sample may leads to a completely different classification results; this effect is known
 2141 as *overtraining*.

2142 An alternative to reduce the overtraining in BDTs consists in pruning the tree
 2143 by removing statistically insignificant nodes after the tree growing is completed but
 2144 this option is not available for BDTs with gradient boosting in the TMVA-toolkit,
 2145 therefore, the overtraining has to be reduced by tuning the algorithm, number of
 2146 nodes, minimum number of events in the leaves, etc. The overtraining can be evaluated
 2147 by comparing the responses of the classifier when running over the training and
 2148 test samples.

2149 5.1.4 Variable ranking

2150 BDTs have a couple of particular advantages related to the input variables; they are
 2151 relatively insensitive to the number of input variables used in the vector \mathbf{x} . The
 2152 ranking of the BDT input variables is determined by counting the number of times a
 2153 variable is used to split decision tree nodes; in addition, the separation gain-squared
 2154 achieved in the splitting and the number of events in the node are accounted by
 2155 applying a weighting to that number. Thus, those variables with small or no power
 2156 to separate signal and background events are rarely chosen to split the nodes, i.e., are
 2157 effectively ignored.

2158 In addition, variables correlations play an important role for some MVA methods
 2159 like the Fisher discriminant algorithm in which the first step consist of performing a
 2160 linear transformation to a phase space where the correlations between variables are
 2161 removed; in the case of BDT algorithm, correlations do not affect the performance.

2162 5.1.5 BDT output example

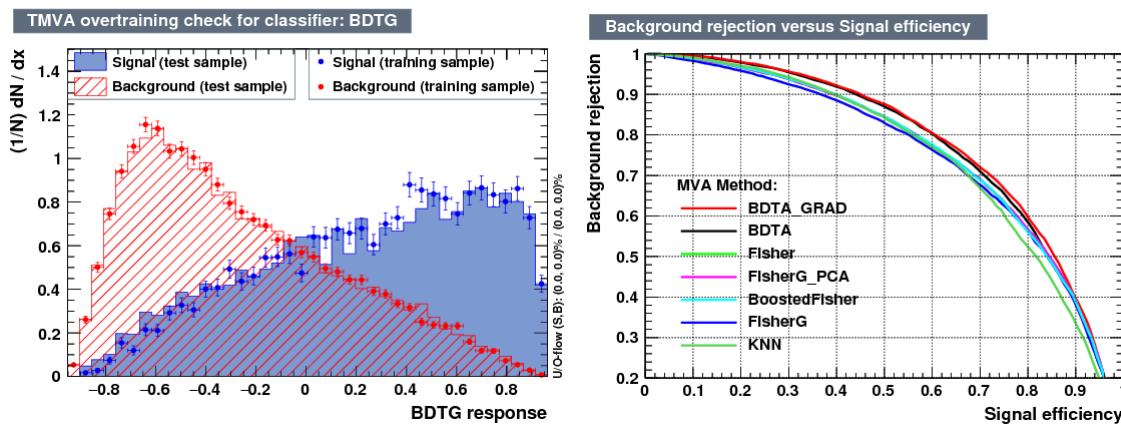


Figure 5.5: Left: Output distributions for the gradient boosted decision tree (BDTG) classifier using a sample of signal ($pp \rightarrow tHq$) and background ($pp \rightarrow tt$) events. Right: Background rejection vs signal efficiency (ROC curves) for various MVA classifiers running over the same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

2163 The left side of figure 5.5 shows the BDT output distributions for signal ($pp \rightarrow$
 2164 tHq) and background ($pp \rightarrow t\bar{t}$) events; this plot is the equivalent to the one showed
 2165 in Figure 5.2. A forest with 800 trees, maximum depth per tree = 3, and gradient
 2166 boosting have been used as training parameters. The BDTG classifier offers a good
 2167 separation power. There is a small overtraining in the signal distribution, while the
 2168 background distribution is very well predicted which might indicate that the sample
 2169 is composed of more background than signal events.

2170 The right side of figure 5.5 shows the background rejection vs signal efficiency
 2171 curves for several combinations of MVA classifiers-boosting algorithms running over
 2172 the same MC sample; these curves are known as ROC curves and give an indication
 2173 of the performance of the classifier. In this particular example, the best performance
 2174 is achieved with the BDTG classifier (BDTA_GRAD), which motivate its use in this
 2175 thesis.

2176 **5.2 Statistical inference**

2177 Once events are classified, the next step consists of finding the parameters that define
 2178 the likelihood functions $f(\mathbf{x}|s)$, $f(\mathbf{x}|b)$ for signal and background events respectively.
 2179 In general, likelihood functions depend not only on the measurements but also on
 2180 parameters (θ_m) that define their shapes; the process of estimating these *unknown*
 2181 *parameters* and their uncertainties from the experimental data is called *inference*.

2182 The statistical inference tools used in this analysis are implemented in the RooFit
 2183 toolkit [132] and COMBINE package [133] included in the CMSSW software frame-
 2184 work.

2185 **5.2.1 Nuisance parameters**

2186 The unknown parameter vector θ is made of two types of parameters: those pa-
 2187 rameters that provide information about the physical observables of interest for the
 2188 experiment or *parameters of interest*, and the *nuisance parameters* that are not of
 2189 a direct interest for the experiment but that need to be included in the analysis in
 2190 order to achieve a satisfactory description of the data; they represent effects of the
 2191 detector response like the finite resolutions of the detection systems, miscalibrations,
 2192 and in general any source of uncertainty introduced in the analysis.

2193 Nuisance parameters can be estimated from experimental data; for instance, data
 2194 samples from a test beam are usually employed for calibration purposes. In cases
 2195 where experimental samples are not availables, the estimation of nuisance parameters
 2196 makes use of dedicated simulation programs to provide the required samples.

2197 The estimation of the unknown parameters involves certain deviations from their
 2198 true values, hence, the measurement of the nuisance parameter is written in terms
 2199 of an estimated value, also called central value, $\hat{\theta}$ and its uncertainty $\delta\theta$ using the
 2200 notation

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

2201 where the interval $[\hat{\theta} - \delta\theta, \hat{\theta} + \delta\theta]$ is called *confidence interval*; it is usually interpreted,
 2202 in the limit of infinite number of experiments, as the interval where the true value
 2203 of the unknown parameter θ is contained with a probability of 0.6827 (if no other
 2204 convention is stated); this interval represents the area under a Gaussian distribution
 2205 in the interval $\pm 1\sigma$.

2206 Conventionally, uncertainties are split into two classes: *systematic*, associated with
 2207 the systematic effects, and *statistical*, related only to fluctuations in data and having

2208 statistical nature.

2209 5.2.2 Maximum likelihood estimation method

2210 The estimation of the unknown parameters that are in best agreement with the ob-
 2211 served data is performed through a function of the data sample that returns the
 2212 estimate of those parameters; that function is called an *estimator*. Estimators are
 2213 usually constructed using mathematical expressions encoded in computer programs.

2214 In this thesis, the estimator used is the likelihood function $f(\mathbf{x}|\boldsymbol{\theta})$ ⁴ which depends
 2215 on a set of measured variables \mathbf{x} and a set of unknown parameters $\boldsymbol{\theta}$. The likelihood
 2216 function for N events in a sample is the combination of all the individual likelihood
 2217 functions, i.e.,

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

2218 and the estimation method used is the *Maximum Likelihood Estimation* method
 2219 (MLE); it is based on the combined likelihood function defined by eqn. 5.10 and
 2220 the procedure seeks for the parameter set that corresponds to the maximum value of
 2221 the combined likelihood function, i.e., the *maximum likelihood estimator* of the un-
 2222 known parameter vector $\boldsymbol{\theta}$ is the function that produces the vector of *best estimators*
 2223 $\hat{\boldsymbol{\theta}}$ for which the likelihood function $L(\boldsymbol{\theta})$ evaluated at the measured \mathbf{x} is maximum.

2224 Usually, the logarithm of the likelihood function is used in numerical algorithm
 2225 implementations in order to avoid underflow the numerical precision of the computers
 2226 due to the product of small likelihoods. In addition, it is common to minimize the
 2227 negative logarithm of the likelihood function, therefore, the negative log-likelihood

⁴ analogue to the likelihood functions described in previous sections

2228 function is

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

2229 The minimization process is performed by the software MINUIT [134] imple-
 2230 mented in the ROOT analysis framework. In case of data samples with large number
 2231 of measurements, the computational resources necessary to calculate the likelihood
 2232 function are too big; therefore, the parameter estimation is performed using binned
 2233 distributions of the variables of interest for which the *binned likelihood function* is
 2234 given by

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

2235 with s_i and b_i the expected number of signal and background yields for the bin i , n_i is
 2236 the observed number of events in the bin i and $r = \sigma/\sigma_{SM}$ is the signal strength. Note
 2237 that the number of entries per bin follows a Poisson distribution. The effect of the
 2238 nuisance parameters have been included in the likelihood function through Gaussian
 2239 distributions that models the nuisance. The three parameters, r , s_i and b_i are jointly
 2240 fitted to estimate the value of r .

2241 5.3 Upper limits

2242 In this analysis, two hypotheses are considered; the background only hypothesis
 2243 ($H_0(b)$) and the signal plus background hypothesis ($H_1(s+b)$), i.e., the sample of
 2244 events is composed of background only events ($r=0$) or it is a mixture of signal plus
 2245 background events ($r=1$). The exclusion of one hypothesis against the other means
 2246 that the observed data sample better agrees with H_0 or rather with H_1 . In order
 2247 to discriminate these hypotheses, a test statistic is constructed on the basis of the

2248 likelihood function evaluated for each of the hypothesis.

2249 The *Neyman-Pearson* lemma [135] states that the test statistic that provides the
 2250 maximum power for H_1 for a given significance level (background misidentification
 2251 probability α), is given by the ratio of the likelihood functions $L(\mathbf{x}|H_1)$ and $L(\mathbf{x}|H_0)$;
 2252 however, in order to use that definition it is necessary to know the true likelihood
 2253 functions, which in practice is not always possible. Approximate functions obtained
 2254 by numerical methods, like the BDT method described above, have to be used, so
 2255 that the *profile likelihood* test statistic is defined by

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

2256 where, \hat{r} and $\hat{\boldsymbol{\theta}}$ maximize the likelihood function, and $\hat{\boldsymbol{\theta}}$ maximizes the likelihood
 2257 function for a given value of the signal strength modifier r . In practice, the test
 2258 statistic t_r

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

2259 is used to evaluate the presence of signal in the sample, since the minimum of t_r at
 2260 $r = \hat{r}$ suggests the presence of signal with signal strength \hat{r} . The uncertainty interval
 2261 for r is determined by the values of r for which $t_r = +1$.

2262 The expected probability density function (p.d.f) $f(t_r|r, \boldsymbol{\theta})$ of the test statistic t_r
 2263 can be obtained numerically by generating MC samples where one hypothesis, $H_0(b)$
 2264 or $H_1(s+b)$, is assumed; thus, MC samples contain the possible values of t_r obtained
 2265 from *pseudo-experiments* as shown in Figure 5.6. The probability that t_r takes a value
 2266 equal or greater than the observed value ($t_{r,obs}$) when a signal with a signal modifier
 2267 r is present in the data sample, is called the *p-value* of the observation; it can be
 2268 calculated using

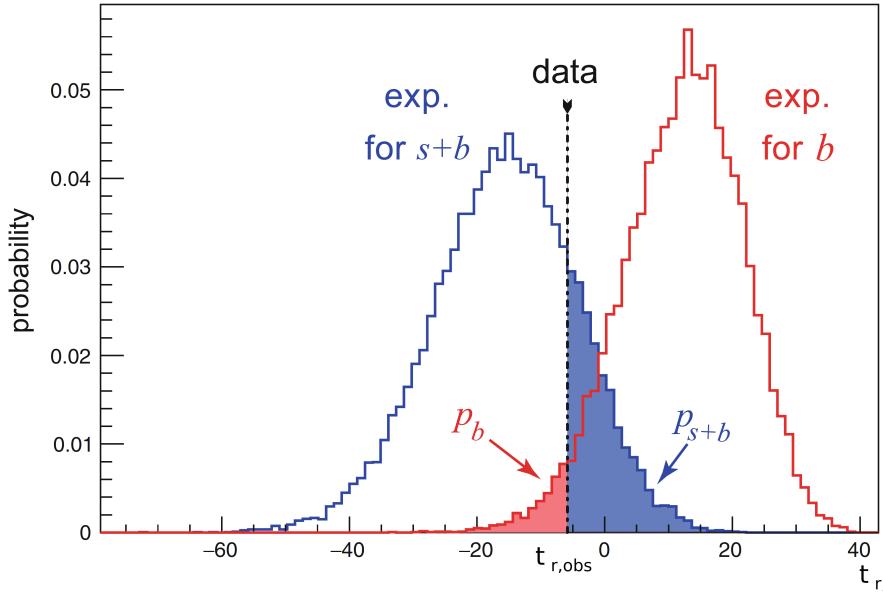


Figure 5.6: t_r p.d.f. from MC pseudo experiments assuming H_0 (red) and H_1 (blue). The black dashed line shows the value of the test statistic as measured from data. Adapted from Reference [128].

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

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

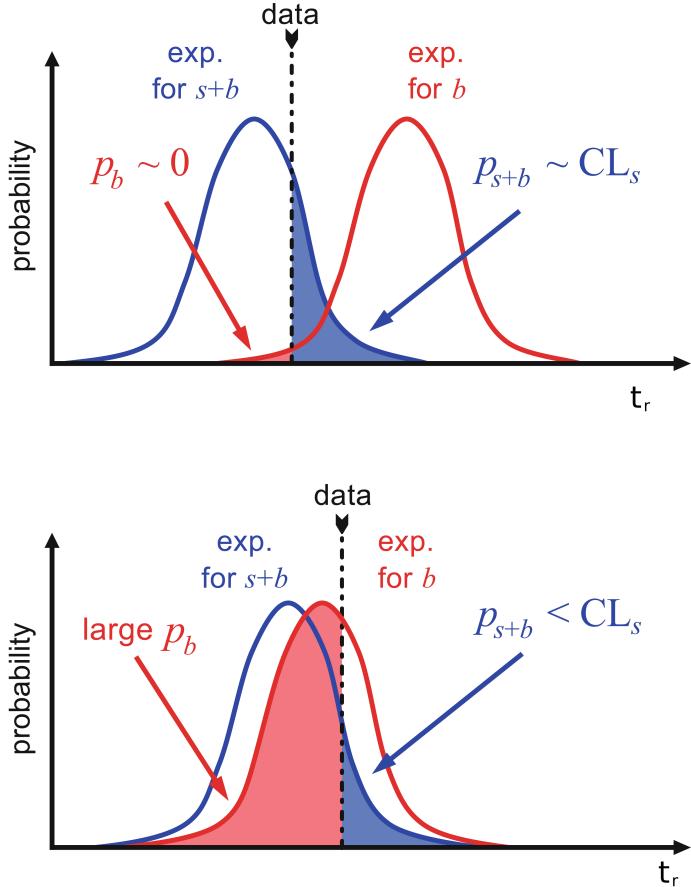


Figure 5.7: CL_s limit illustration. When the test statistic p.d.f. for the two hypotheses H_0 and H_1 are well separated (top) and when they are largely overlapped (bottom). Adapted from Reference [128].

2277 background-only hypothesis. These issues are corrected by using the modified p-
2278 value [136]

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

2279 If H_1 is true, then p_b is small, $CL_s \simeq p_r$ and H_0 is rejected; if there is large
2280 overlap and a statistical fluctuation causes that p_b is large, then both numerator and
2281 denominator in Eqn. 5.17 become small but CL_s would allow the rejection of H_1
2282 even if there is poor sensitivity to signal.

2283 The upper limit of the parameter of interest r^{up} is determined by excluding the
 2284 range of values of r for which $CL_s(r, \theta)$ is lower than the confidence level desired,
 2285 normally 90% or 95%, e.g, scanning over r and finding the value for which $p_r'^{up} =$
 2286 0.05. The expected upper limit can be calculated using pseudo-experiments based on
 2287 the background-only hypothesis and obtaining a distribution for r_{ps}^{up} ; the median of
 2288 that distribution corresponds to the expected upper limit, while the $\pm 1\sigma$ and $\pm 2\sigma$
 2289 deviations correspond to the values of the distribution that defines the 68% and 95%
 2290 of the area under the distribution centered in the median. It is usual to present all
 2291 the information about the expected and observed limits in the so-called *Brazilian-flag*
 2292 plot as the one showed in Figure 5.8. The solid line represent the observed CL_s

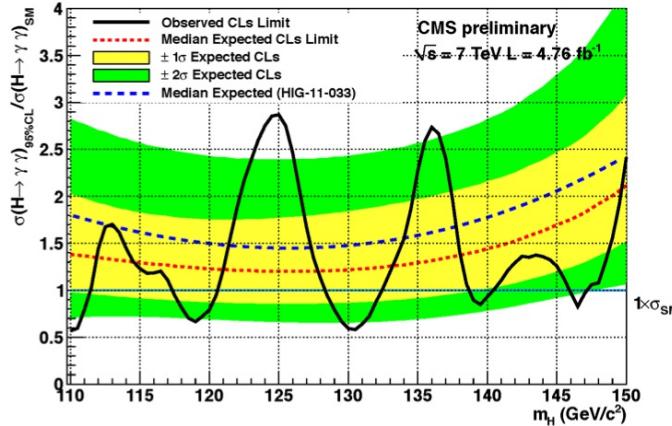


Figure 5.8: Brazilian flag plot of CMS experiment limits for Higgs boson decaying to photons [137].

2293 5.4 Asymptotic limits

2294 As said before, the complexity of the likelihood functions, the construction of test
 2295 statistics, and the calculation of the limits and their uncertainties is not always man-
 2296 ageable and requires extensive computational resources; in order to overcome those
 2297 issues, asymptotic approximations for likelihood-based test statistics, like the ones

2298 described in previous sections, have been developed [138, 139] using Wilks' theorem.
2299 Asymptotic approximations replace the construction of the test statistics p.d.f.s using
2300 MC pseudo-experiments, with the approximate calculation of the test statistics p.d.f.s
2301 by employing the so-called *Asimov dataset*.

2302 The Asimov dataset is defined as the dataset that produce the true values of the
2303 nuisance parameters when it is used to evaluate the estimators for all the parameters;
2304 it is obtained by setting the values of the variables in the dataset to their expected
2305 values [139].

2306 Limits calculated by using the asymptotic approximation and the Asimov dataset
2307 are know as *asymptotic limits*.

2308 **Chapter 6**

2309 **Search for production of a Higgs**

2310 **boson and a single top quark in**

2311 **multilepton final states in pp**

2312 **collisions at $\sqrt{s} = 13$ TeV**

2313 **6.1 Introduction**

2314 The Higgs boson discovery, supported on experimental observations and theoretical

2315 predictions made about the SM, gives the clue of the way in that elementary parti-

2316 cles acquire mass through the Higgs mechanism; therefore, knowing the Higgs mass,

2317 the Higgs-vector boson and Higgs-fermion couplings can be tested. In order to test

2318 the Higgs-top coupling, several measurements have been performed, as stated in the

2319 chapter 1, but they are limited in sensitivity to measure the square of the coupling.

2320 The production of a Higgs boson in association with a single top quark (tH) not

2321 only offers access to the sign of the coupling, but also, to the CP phase of the Higgs

2322 couplings.

2323 This chapter presents the search for the associated production of a Higgs boson
 2324 and a single top quark (tHq) events, focusing on leptonic signatures provided by the
 2325 Higgs decay modes to WW , ZZ , and $\tau\tau$; the 13 TeV dataset produced in 2016, with
 2326 an integrated luminosity of 35.9fb^{-1} , is used.

2327 As shown in Section 1.5, the SM cross section of tHq process is affected by a
 2328 destructive interference between two contributions (see Figure 1.15), where the Higgs
 2329 couples to either the W boson or the top quark; however, if the sign of the Higgs-
 2330 top coupling is flipped with respect to the SM prediction, a large enhancement of
 2331 the cross section occurs, making this analysis sensitive to such deviation. A second
 2332 process, where the Higgs boson and top quark are accompanied by a W boson (tHW)
 2333 has similar behavior, albeit with a weaker interference pattern and lower contribution
 2334 to the cross section, therefore, a combination of both processes would increase the
 2335 sensitivity to the sign of the coupling; in this analysis both contributions are combined
 2336 and referred to as tH channel. A third contribution comes from $t\bar{t}H$ process. The
 2337 purpose of this analysis is to investigate the exclusion of the presence of the $tH+$
 2338 $t\bar{t}H$ processes in the SM under the assumption of the anomalous Higgs-top coupling
 2339 modifier ($\kappa_t = -1$). The analysis exploits signatures with two leptons of the same sign
 2340 ($2lss$) channel and three leptons ($3l$) channel in the final state.

2341 Constraints on the sign of the Higgs-top coupling (y_t) have been derived from the
 2342 decay rate of Higgs boson to photon pairs [50] and from the cross section for associated
 2343 production of Higgs and Z bosons via gluon fusion [141], with recent results disfavoring
 2344 negative signs of the coupling [44, 59, 142], although the negative sign coupling have
 2345 not been completely excluded.

2346 The analysis presented here, expands previous analyses performed at 8 TeV [143,
 2347 144] and searches for associated production of $t\bar{t}$ pair and a Higgs boson in the mul-

2348 tilepton final state channel [145]; it also complements searches in $H \rightarrow b\bar{b}$ [146].

2349 The first sections present the characteristic tHq signature as well as the expected
 2350 backgrounds. The MC samples, data sets, and the physics object definitions are then
 2351 described; after, the background predictions, the signal extraction, the statistical
 2352 treatment of the selected events and the discussion of the systematic uncertainties
 2353 are described. The final section present the results for the exclusion limits as a
 2354 function of the ratio of κ_t and the dimensionless modifier of the Higgs-vector boson
 2355 coupling κ_V .

2356 The analysis is designed to efficiently identify and select prompt leptons from on-
 2357 shell W and Z boson decays and to reject non-prompt leptons from b quark decays
 2358 and spurious lepton signatures from hadronic jets. Events are then selected in the
 2359 $2lss$ and $3l$ channels, and are required to contain hadronic jets, some of which must
 2360 be consistent with b quark hadronization. Finally, the signal yield is extracted by
 2361 simultaneously fitting the output of two dedicated multivariate discriminants, trained
 2362 to separate the tHq signal from the two dominant backgrounds, in all categories. The
 2363 fit result is then used to set an upper limit on the combined $t\bar{t}H + tH$ production
 2364 cross section, as a function of the relative coupling strengths of Higgs-top quark and
 2365 Higgs-Vector boson. Figure 6.1 shows an schematic overview of the analysis strategy
 2366 workflow.

2367 With respect to the 8 TeV analysis, the object selections have been adjusted for
 2368 the updated LHC running conditions at 13 TeV, the lepton identification has been
 2369 improved, and more powerful multivariate analysis techniques are used for the signal
 2370 extraction.

2371 The analysis has been made public by CMS as a Physics Analysis Summary [147]
 2372 combining the result for the three lepton and two lepton same-sign channels; the
 2373 content present in this chapter is based on that document and on References [145,149]

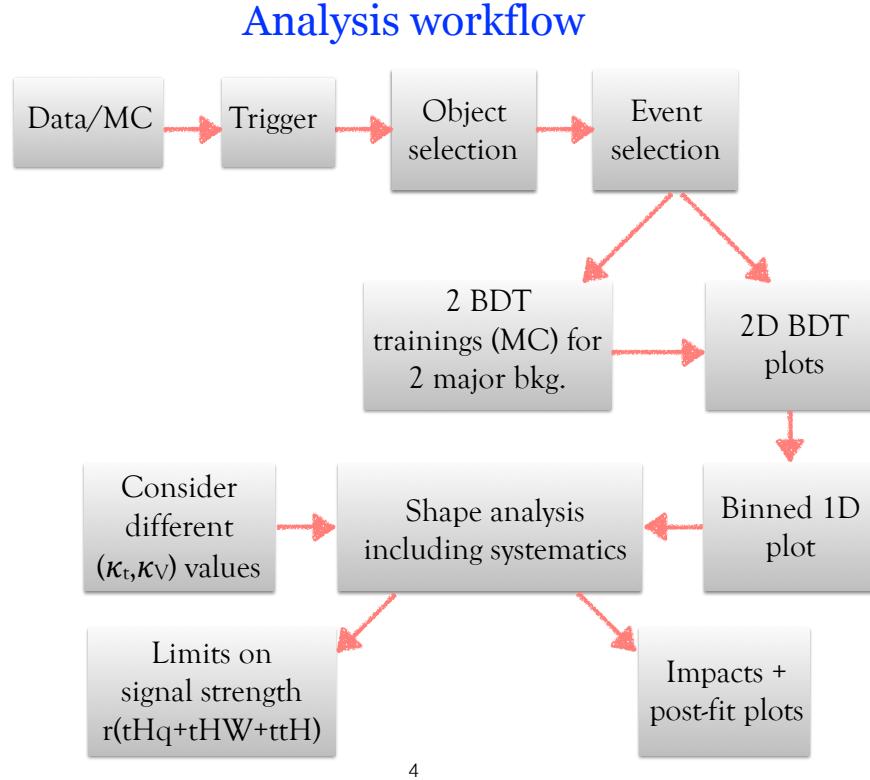


Figure 6.1: A schematic overview of the analysis workflow. Based on sets of optimized physics object definitions and selection criteria, signal and background events in a data sample are discriminated. The discrimination is performed by a BDT, previously trained using MC samples of the dominant backgrounds,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

2374 unless other Reference is stated. Currently, an effort to turn the analysis into a paper
 2375 combining the multilepton and $H \rightarrow b\bar{b}$ is ongoing.

2376 6.2 tHq signature

2377 In order to select events of tHq process, its features are translated into a set of
 2378 selection rules; Figure 6.2 shows the Feynman diagram and a schematic view of the

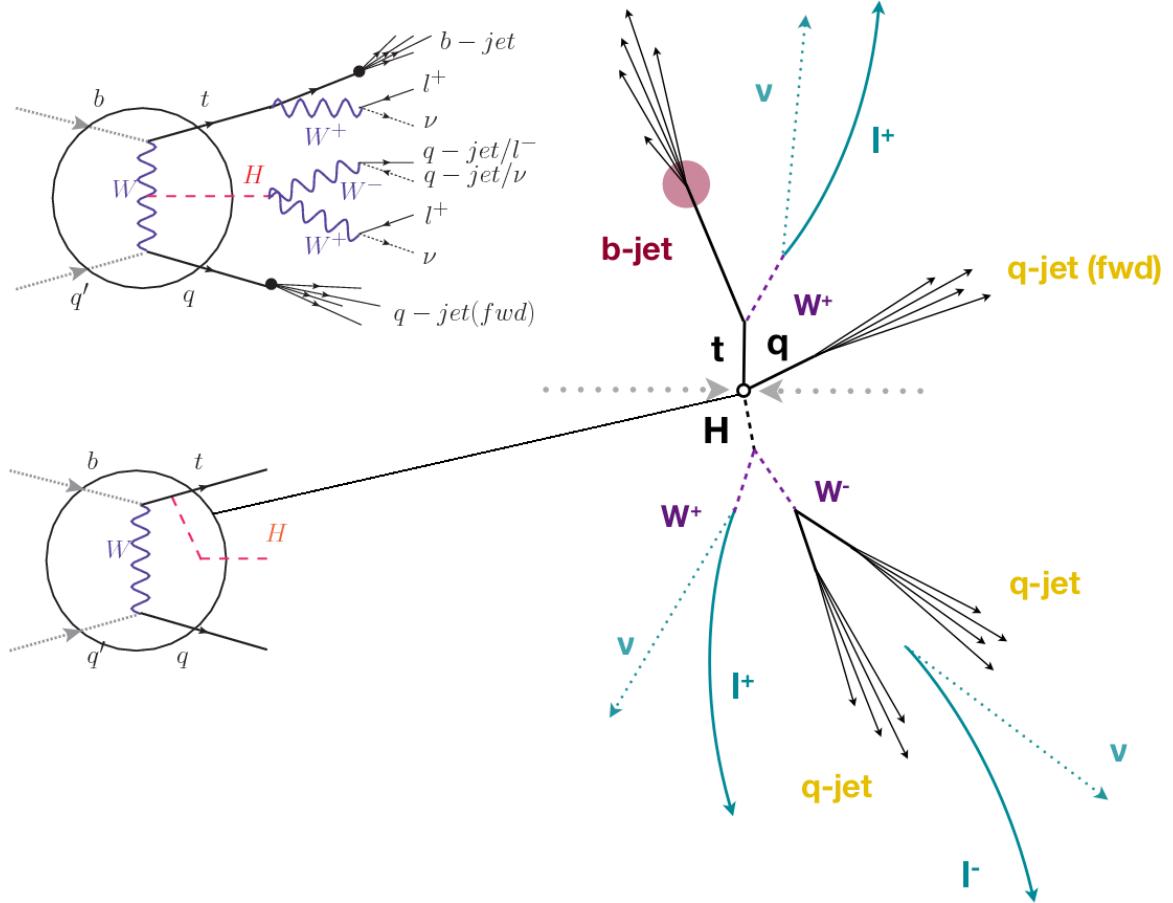


Figure 6.2: tHq event signature. Left: Feynman diagram including the whole evolution up to the final state for the case of the Higgs boson emitted by the W boson (top); Feynman diagram for the case where the Higgs boson is emitted by the top quark. Right: Schematic view as it would be seen in the detector; 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.

2379 tHq process from the pp collision to the final state configuration. A single top quark
 2380 is produced accompanied by a light quark, denoted as q ; this light quark is produced
 2381 predominantly in the forward region of the detector. The Higgs boson can be either
 2382 emitted by the exchanged W boson or directly by the singly produced top quark.

2383 Due to their high masses/short lifetimes, top quark and Higgs boson decay after
 2384 their production within the detector. The Higgs boson is required to decay into a W

2385 boson pair¹. The top quark almost always decays into a bottom quark and a W boson,
 2386 as encoded in the CMK matrix. The W bosons are required to decay leptonically
 2387 either all the three in the $3l$ channel or the pair with equal electrical charge in the
 2388 $2lss$ channel case; τ leptons are not reconstructed separately and only their leptonic
 2389 decays into either electrons or muons are considered in this analysis.

2390 In summary, the signal process is characterized by a the final state with

- 2391 • one light-flavored forward jet,
 - 2392 • one central b-jet,
 - 2393 • $2lss$ channel \rightarrow two leptons of the same sign, two neutrinos and two light (often
 2394 soft) jets,
 - 2395 • $3l$ channel \rightarrow three leptons, three neutrinos and no central light-flavored jets,
- 2396 The presence of neutrinos is inferred from the presence of MET.

2397 6.3 Background processes

2398 The background processes are those that can mimic the signal signature or at least
 2399 can be reconstructed as that as a result of certain circumstances. The backgrounds
 2400 can be classified as

- 2401 • irreducible backgrounds: where genuine prompt leptons are produced in on-
 2402 shell W and Z boson decays; they can be reliably estimated directly from MC
 2403 simulated events, using higher-order cross sections or data control regions for
 2404 the overall normalization.

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

2405 • reducible backgrounds: where at least one of the leptons is *non-prompt*, i.e.,
 2406 produced within a hadronic jet; genuine leptons from heavy flavor decays and
 2407 misreconstructed jets, also known as *mis-ID leptons* are considered non-prompt
 2408 leptons or or *fake leptons* as well as electrons from photon conversions. These
 2409 non-prompt leptons leave tracks and hits in the detection systems as would a
 2410 prompt lepton, but evaluation the correlation of those hits with nearby jets
 2411 could be a way of removing them. The misassignment of electron charge in
 2412 processes like $t\bar{t}$ or Drell-Yan, represent an additional source of background,
 2413 but it is relevant only for the $2lss$ channel. Reducible backgrounds are not well
 2414 predicted by simulation, hence, they are estimated using data-driven methods.

2415 The main sources of background events for tHq process are $t\bar{t}$ process and $t\bar{t}V(V =$
 2416 W, Z, γ) processes. Figure 6.3 shows the signature for $t\bar{t}$ and $t\bar{t}W$ processes.

2417 The largest contribution to irreducible backgrounds comes from $t\bar{t}W$ and $t\bar{t}Z$ processes
 2418 for which the number of ($b-$)jets (($b-$)jet multiplicity) is higher than that of the sig-
 2419 nal events, while for other contributing background events, WZ , ZZ , and rare SM
 2420 processes like $W^\pm W^\pm qq$, $t\bar{t}t\bar{t}$, tZq , tZW , WWW , WWZ , WZZ , ZZZ , the ($b-$)jet
 2421 multiplicity is lower compared to that of the signal events. None of the irreducible
 2422 backgrounds present activity in the forward region of the detector.

2423 On the side of the reducible backgrounds, the largest contribution comes from the
 2424 $t\bar{t}$ events which have a very similar signature to the signal events but does no present
 2425 activity in the forward region of the detector either; A particular feature of the $t\bar{t}$
 2426 events is their charge-symmetry, which is different from the characteristics of signal
 2427 events.

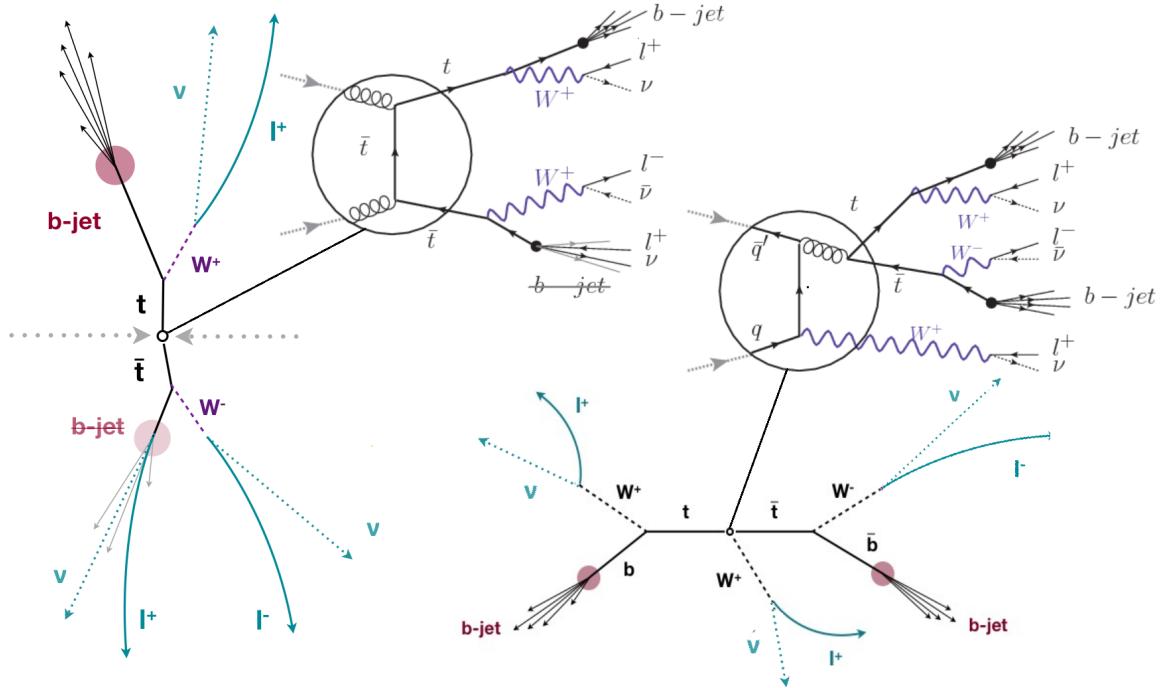


Figure 6.3: $t\bar{t}$ (left) and $t\bar{t}W$ (right) events signature as they would be seen in the detector; the Feynman diagrams including the whole evolution up to the final state are also showed. The $t\bar{t}$ process signature is very similar to that of the signal process with one fake lepton and non 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.

2428 6.4 Data and MC Samples

2429 6.4.1 Full 2016 data set

2430 The data set used in this analysis was collected by the CMS experiment during 2016
 2431 at while running at $\sqrt{s} = 13\text{TeV}$ and corresponds to a total integrated luminosity
 2432 of 35.9fb^{-1} . Only periods when the CMS magnet was on were considered when
 2433 selecting the data samples; that corresponds to the 23Sep2016 (Run B to G) and
 2434 PromptReco (Run H) versions of the datasets.

2435 Multilepton final states with either two same-sign leptons or three leptons tar-
 2436 get the case where the Higgs boson decays to a pair of W bosons, τ leptons, or Z
 2437 bosons, and where the top quark decays leptonically, hence, the SingleElectron,

2438 SingleMuon, DoubleEG, MuonEG, DoubleMuon dataset (see Table A.1) compose the
 2439 full dataset. The certified luminosity sections are selected using the golden JSON file
 2440 defined by the CMS experiment [148].

2441 6.4.2 Triggers

2442 The events considered are those online-reconstructed events triggered by one, two, or
 2443 three leptons. Single-lepton triggers are included in order to boost the acceptance
 2444 of events where the p_T of the sub-leading lepton falls below the threshold of the
 2445 double-lepton triggers. The trigger efficiency is increased by including double-lepton
 2446 triggers in the $3l$ category, and single-lepton triggers in all categories; it is possible
 2447 given the logical “or” of the trigger decisions of all the individual triggers in a given
 2448 category. Table A.2 shows the lowest-threshold non-prescaled triggers present in the
 2449 High-Level Trigger (HLT) menus for both Monte-Carlo and data in 2016.

2450 Trigger efficiency scale factors

2451 Trigger efficiency describes the ability of events to pass the trigger requirements. It
 2452 is measured in simulated events using generator information given that there is no
 2453 trigger bias with the MC sample. Measuring the trigger efficiency in data requires a
 2454 more elaborated procedure; first, select a set of events collected by a trigger that is
 2455 uncorrelated with the lepton triggers such that the selected events form an unbiased
 2456 sample. In this analysis, that uncorrelated trigger is a MET trigger. Second step
 2457 is looking for candidate events with exactly two good leptons (exactly three good
 2458 leptons for the $3l$ channel). Finally, measure the efficiency for the candidate events to
 2459 pass the logical “or” of triggers being considered in a given event category as defined
 2460 in Table A.2.

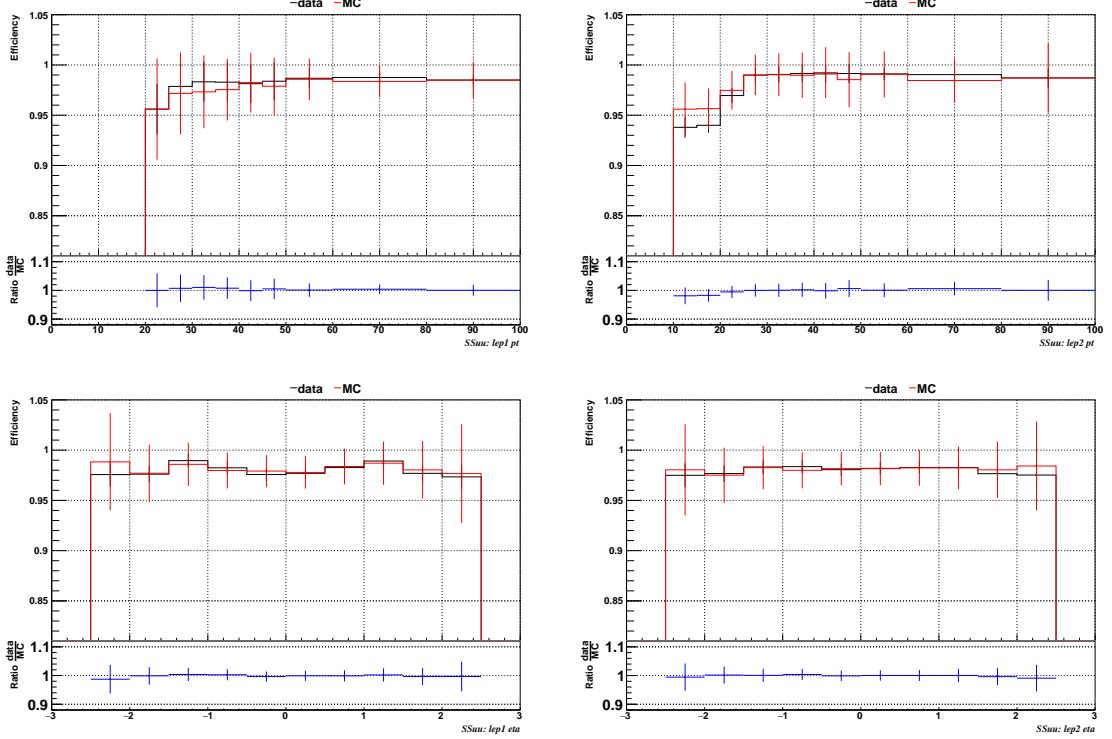


Figure 6.4: Comparison between data and MC trigger efficiencies in the same-sign $\mu\mu$ category, as a function of the p_T (top) and η (bottom) of the leading lepton (left) and the sub-leading lepton (right) [149].

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

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

2461 Comparisons between the data and MC efficiencies for each category, showed in
 2462 Figures 6.4, 6.5, and 6.6, reveal that they are in good agreement; the difference is
 2463 corrected by applying scale factors derived from the ratio between both efficiencies.
 2464 Applied flat scale factors in each category are shown in Table 6.1; they have been
 2465 inherited from Reference [149].

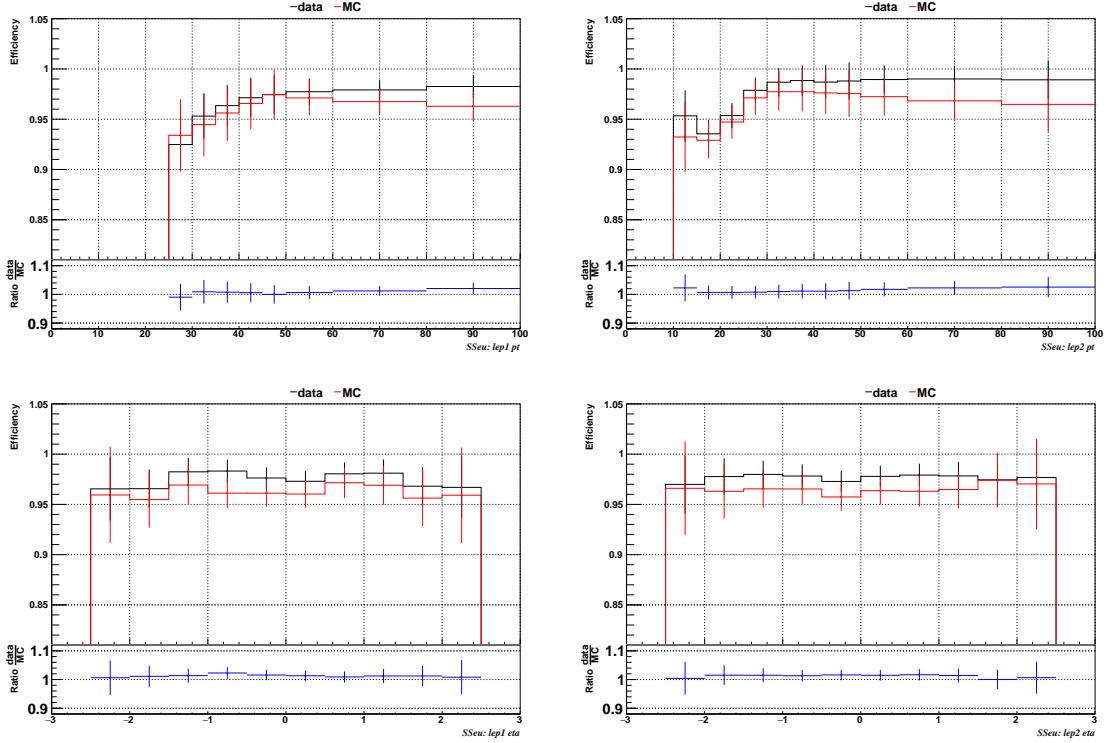


Figure 6.5: Comparison between data and MC trigger efficiencies in the same-sign $e\mu$ category as a function of the p_T (top) and η (bottom) of the leading lepton (left) and the sub-leading lepton (right) [149].

2466 6.4.3 MC samples

2467 Current event generators allow the adjustment of the kinematics of the generated
 2468 events, based on an event-wise reweighting; in this way, several generation parameters
 2469 phase spaces can be explored according to the experimental interests. The signal
 2470 samples used in this analysis were generated in such a way that not only the case κ_t
 2471 $= -1$, but an extended range of κ_t and κ_V values may be investigated.

2472 tHq and tHW cross section in the κ_t - κ_V phase space are shown in Figure 6.7. As
 2473 said in section 3.1, the tHq sample was generated using the 4F scheme which provides
 2474 a better description of the additional b quark from the initial gluon splitting, while the
 2475 tHW sample was generated using the 5F scheme in order to remove its interference

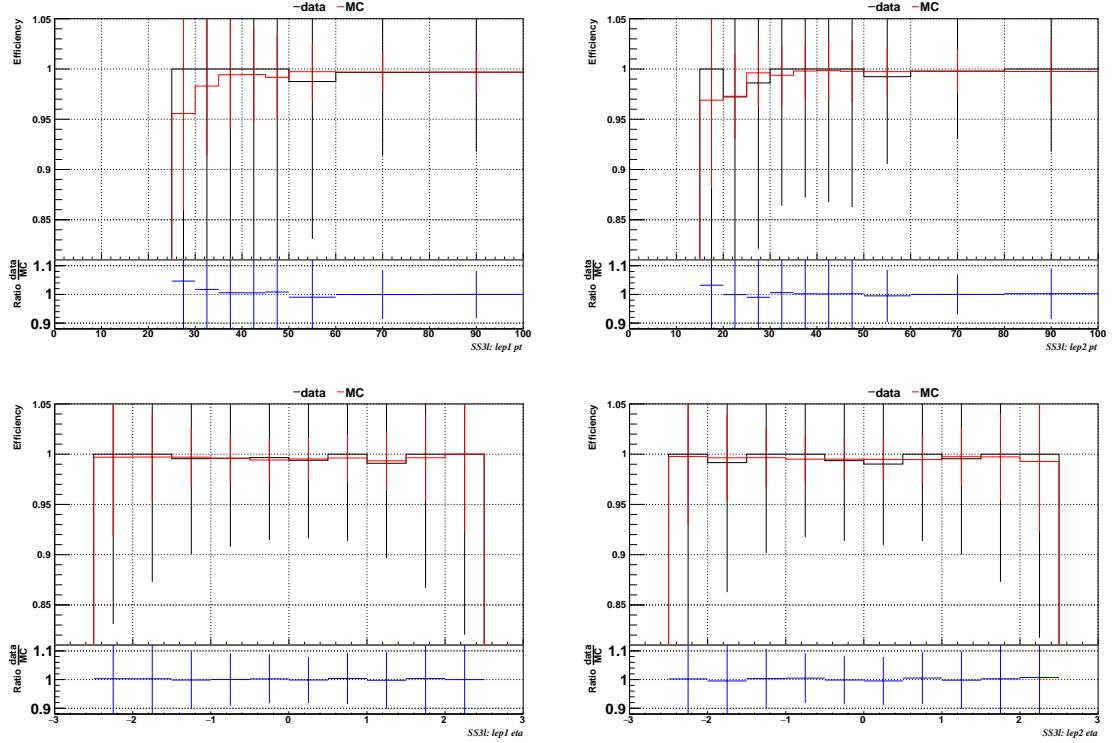


Figure 6.6: Comparison between data and MC trigger efficiencies in the $3l$ category, as a function of the p_T (top) and η (bottom) of the leading lepton (left) and the sub-leading lepton (right) [149].

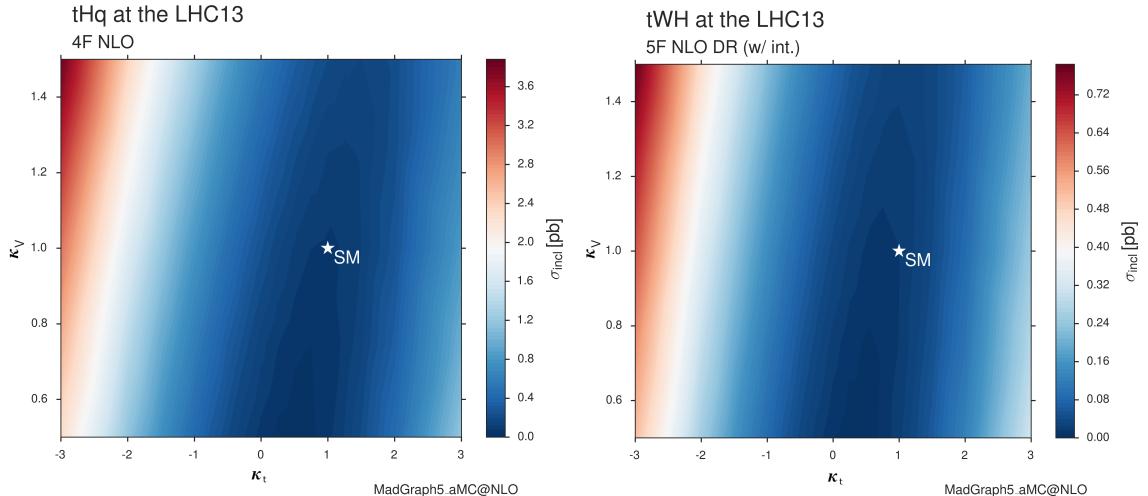


Figure 6.7: tHq and tHW cross section in the κ_t - κ_V phase space [150].

2476 with $t\bar{t}H$ at LO.

2477 MC signal samples

2478 The two signal samples, tHq and tHW , correspond to the RunIISummer16MiniAODv2
 2479 campaign produced with CMSSW_80X; they were produced with MG5_aMC@NLO
 2480 (version 5.2.2.3), in LO mode at $\sqrt{s} = 13$ TeV, and are normalized to NLO cross sec-
 2481 tions (see Table 6.2). The Higgs boson is assumed to be SM-like except for the values
 2482 of its couplings to the top quark and W boson. Each sample was generated with a set
 2483 of event weights corresponding to 51 different values of (κ_t, κ_V) couplings, accessible
 2484 in terms of LHE event weights as shown in Table A.3; however, the main interest is
 2485 the $(\kappa_t = -1, \kappa_V = 1)$ case.

Sample	σ [pb]	BF
/THQ_Hincl_13TeV-madgraph-pythia8_TuneCUETP8M1/	0.7927	0.324
/THW_Hincl_13TeV-madgraph-pythia8_TuneCUETP8M1/	0.1472	1.0
/tTHJetToNonbb_M125_13TeV_amcatnloFXFX_madspin_pythia8_mWCutfix/	0.2151	1.0

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

2486 The $t\bar{t}H$ sample was produced using AMC@NLO interfaced to PYTHIA 8 for
 2487 the parton shower, and is scaled to NLO cross sections. The $t\bar{t}H$ cross section depends
 2488 quadratically on κ_t ; however, in contrast to the tHq and tHW samples, the scaling
 2489 is not performed during the sample generation process but in the analysis code since
 2490 it was decided to include the $t\bar{t}H$ process as a part of the signal in the course of the
 2491 analysis.

2492 MC background samples

2493 Several MC generators were used to generate the samples of the background processes.
 2494 The dominant background sources ($t\bar{t}$, $t\bar{t}W$, $t\bar{t}Z$) were produced using AMC@NLO

2495 interfaced to PYTHIA8, and are scaled to NLO cross sections. Other minor back-
 2496 ground processes are simulated using POWHEG interfaced to PYTHIA, or bare
 2497 PYTHIA as stated in the sample names in Table A.4. Pileup interactions are in-
 2498 cluded in the simulation in order to reflect the observed multiplicity in data; the
 2499 simulated events are weighted according to the actual pileup in data, estimated from
 2500 the measured bunch-to-bunch instantaneous luminosity and the total inelastic cross
 2501 section, 69.2 mb. All events are finally passed through a full simulation of the CMS
 2502 detector using GEANT4, and reconstructed using the same algorithms as used for
 2503 the data.

2504 6.5 Object Identification

2505 In this section, the specific definitions of the physical objects in terms of the recon-
 2506 struction parameters are presented; thus, the provided details summarize and com-
 2507 plement the descriptions presented in previous chapters. The object reconstruction
 2508 and selection strategy used in this thesis are inherited from the analyses in Refer-
 2509 ences [145, 149].

2510 6.5.1 Lepton reconstruction and identification

2511 Two types of leptons are defined in this analysis: *signal leptons* are those coming from
 2512 W, Z and τ decays which usually are isolated from other particles; *background leptons*
 2513 are defined as leptons produced in b -jet hadron decays, light-jets misidentification,
 2514 and photon conversions.

2515 The process of reconstruction and identification of electron and muon candidates
 2516 was described in chapter 3, hence, the identification variables used in order to retain

2517 the highest possible efficiency for signal leptons while maximizing the rejection of
 2518 background leptons are listed and described in the following sections ².

2519 The identification variables include not only observables related directly to the re-
 2520 constructed leptons themselves, but also to the clustered energy deposits and charged
 2521 particles in a cone around the lepton direction (jet-related variables); an initial loose
 2522 preselection of leptons candidates is performed and then an MVA discriminator, re-
 2523 ferred to as *lepton MVA* discriminator, is used to distinguish signal leptons from
 2524 background leptons.

2525 Muons

2526 The Physics Objects Groups (POG) at CMS, are in charge of studying and defining
 2527 the set of selection criteria applied on the course of reconstruction and identification
 2528 of particles. These selection criteria are implemented in the CMS framework in the
 2529 form of several object identification working points according to the strength of the
 2530 requirements.

2531 The muon candidates are reconstructed by combining information from the tracker
 2532 system and the muon detection system of CMS detector and the POG defined three
 2533 working points for muon identification *MuonID* [153];

- 2534 • *POG Loose Muon ID* is a particle identified as a muon by the PF event re-
 2535 construction and also reconstructed either as a global-muon or as an arbitrated
 2536 tracker-muon. This identification criteria is designed to be highly efficient for
 2537 prompt muons and for muons from heavy and light quark decays; it can be com-
 2538 plemented by applying impact parameter cuts in analyses with prompt muon
 2539 signals.

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

- 2540 • *POG Medium Muon ID* is a Loose muon with additional track-quality and
 2541 muon-quality (spatial matching between the individual measurements in the
 2542 tracker and the muon system) requirements. This identification criteria is de-
 2543 signed to be highly efficient in the separation of the muons coming from decay
 2544 in flight of heavy quarks and muons coming from B meson decays as well as
 2545 prompt muons. An additional category *MVA Prompt ID* is defined in this iden-
 2546 tification criteria directed to discriminated muons from B mesons and prompt
 2547 muons (from W,Z and τ decays). The Medium ID provides the same fake rate as
 2548 the Tight Muon ID but a higher efficiency on prompt and B-decays muons. [154]
- 2549 • *POG Tight Muon ID* is a global muon with additional muon-quality require-
 2550 ments Tight Muon ID selects a subset of the PF muons.

2551 Only muons within the muon system acceptance $|\eta| < 2.4$ and minimum p_T of 5
 2552 GeV are considered.

2553 **Electrons**

2554 Electrons are reconstructed using information from the tracker and from the electro-
 2555 magnetic calorimeter and identified by an MVA algorithm (*MVA eID* discriminant)
 2556 using the shape of the calorimetric shower variables like the shape in η and ϕ , the clus-
 2557 ter circularity, widths along η and ϕ ; track-cluster matching variables like E_{tot}/p_{in} ,
 2558 E_{Ele}/p_{out} , $\Delta\eta_{in}$, $\Delta\eta_{out}$, $\Delta\phi_{in}$, $1/E - 1/p$; and track quality variables like χ^2 of the
 2559 GSF tracks, the number of hits used by the GSF filter [155].

2560 A loose selection based on η -dependent cuts on this discriminant is used to prese-
 2561 lect electron candidates, the full shape of the discriminant is used in the lepton MVA
 2562 selection to separate signal leptons from background leptons (described in Section
 2563 6.5.1).

2564 In order to reject electrons from photon conversions, electron candidates with
 2565 missing hits in the pixel tracker layers or matched to a conversion secondary vertex
 2566 are discarded. Electrons are selected for the analysis if they have $p_T > 7$ GeV and
 2567 are located within the tracker system acceptance region ($|\eta| < 2.5$).

2568 **Lepton vertexing and pile-up rejection**

2569 The impact parameter in the transverse plane d_0 , impact parameter along the z -
 2570 axis d_z , and the impact parameter significance in the detector space SIP_{3D} , are
 2571 considered to perform the identification and rejection of pile-up, misreconstructed
 2572 tracks, and background leptons from b-hadron decays; pile-up and misreconstructed
 2573 track mitigation is achieved by imposing loose cuts on the impact parameter variables.
 2574 The full shape of those variables is used in a lepton MVA classifier to achieve the
 2575 best separation between the signal and the background leptons.

2576 **Lepton isolation**

2577 PF is able to recognize leptons from two different sources: on one side, leptons from
 2578 the decays of heavy particles, such as W and Z bosons, which are normally isolated
 2579 in space from the hadronic activity in the event; on the other side, leptons from the
 2580 decays of hadrons and jets misidentified as leptons, which are not isolated as the
 2581 former. For highly boosted systems, like the lepton and the b -jet generated in the
 2582 semileptonic decay of a boosted top, the decay products tend to be more closer and
 2583 sometimes they even overlap; thus, the PF standard definition of isolation in terms
 2584 of the separation between the lepton candidates (l) and other PF objects (i) in the
 2585 η - ϕ 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 ρ is the pileup energy density, h^\pm, h^0, γ, 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.

2600 **Jet-related variables**

2601 In order to reject misidentified leptons from b -jets, mostly coming from $t\bar{t}$ +jets,
 2602 Drell-Yan+jets, and W +jets events, the vertexing and isolation described in previous
 2603 sections are complemented with additional variables related to the closest recon-
 2604 structed jet to the lepton, i.e., the PF jets reconstructed³ around the leptons with
 2605 $\Delta R = \sqrt{(\eta^l - \eta^{jet})^2 + (\phi^l - \phi^{jet})^2} < 0.5$. The identification variables used in the lep-
 2606 ton MVA discriminator are the ratio p_T^l/p_T^{jet} , the CSV b-tagging discriminator value
 2607 of the jet, the number of charged tracks of the jet, and the relative p_T given by

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

2608 **LeptonMVA discriminator**

2609 Electrons and muons passing the basic selection process described above are referred
 2610 to as *loose leptons*. Additional discrimination between signal leptons and background
 2611 leptons is crucial considering that the rate of $t\bar{t}$ production is much larger than the
 2612 signal, hence, an overwhelming background from $t\bar{t}$ production is present. To maxi-
 2613 mally exploit the available information in each event to that end, the dedicated lepton
 2614 MVA discriminator, based on a boosted decision tree (BDT) algorithm, has been built
 2615 so that all the identification variables can be used together.

2616 The lepton MVA discriminator training is performed using simulated signal Loose
 2617 leptons from the $t\bar{t}H$ MC sample and fake leptons from the $t\bar{t}$ +jets MC sample,
 2618 separately for muons and electrons. The input variables used include vertexing, iso-
 2619 lation and jet-related variables, the p_T and η of the lepton, the electron MVA eID
 2620 discriminator and the muon segment-compatibility variables. An additional require-
 2621 ment known as *tight-charge* requirement, is imposed by comparing two independent

³ 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^{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 η 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 (value₁, value₂, value₃). For the two p_T^{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.

2647 **6.5.2 Lepton selection efficiency**

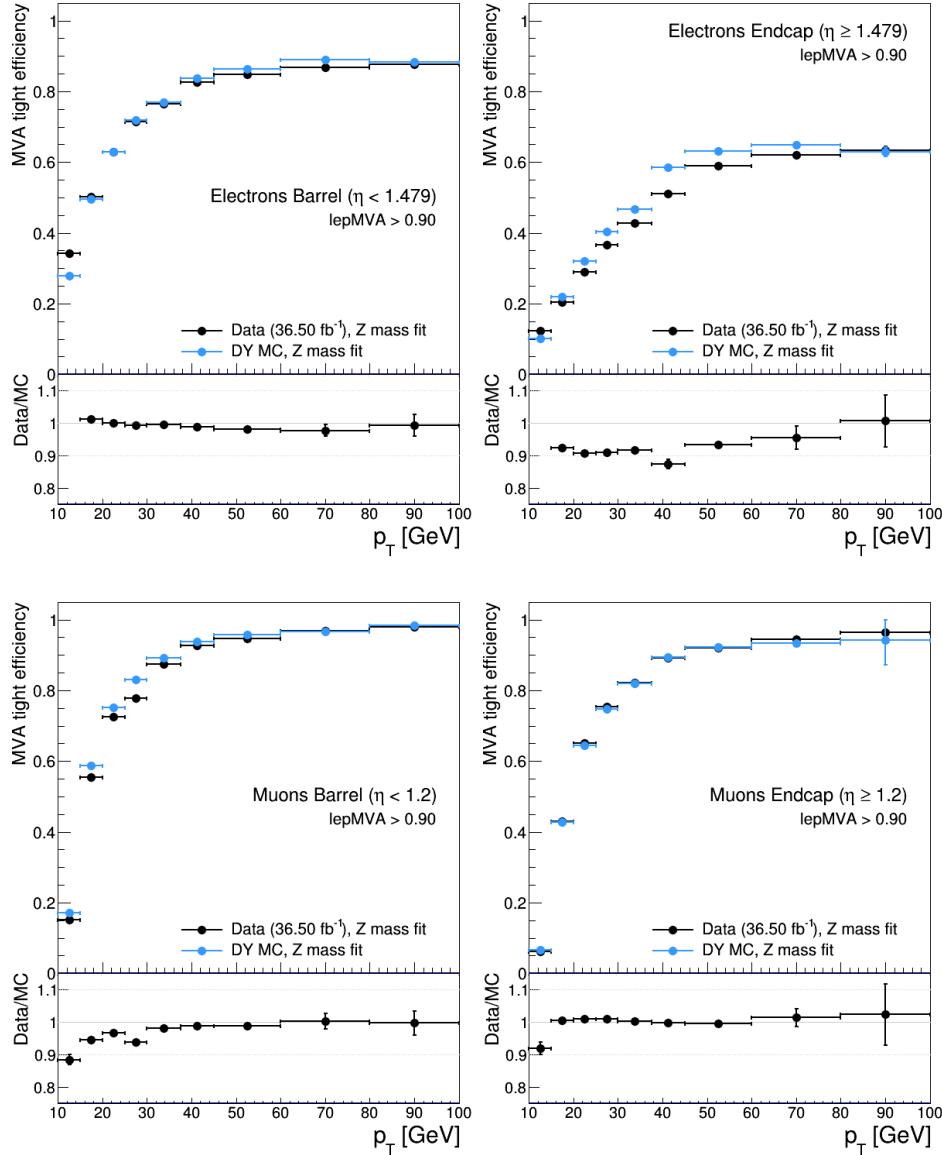


Figure 6.8: Tight vs loose selection efficiencies for electrons (top), and muons (bottom), for the $2lss$ definition, i.e., including the tight-charge requirement.

2648 Efficiencies of reconstruction and selecting loose leptons are measured both for
 2649 muons and electrons using a tag and probe method on both data and MC, using
 2650 $Z \rightarrow \ell^+ \ell^-$ [157]. The scale factors are derived from the ratio of efficiencies $\varepsilon_i(p_T, \eta)$

2651 measured for a given lepton in data/MC, according to

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

2652 The scale factor for each event is used to correct the weight of the event in the

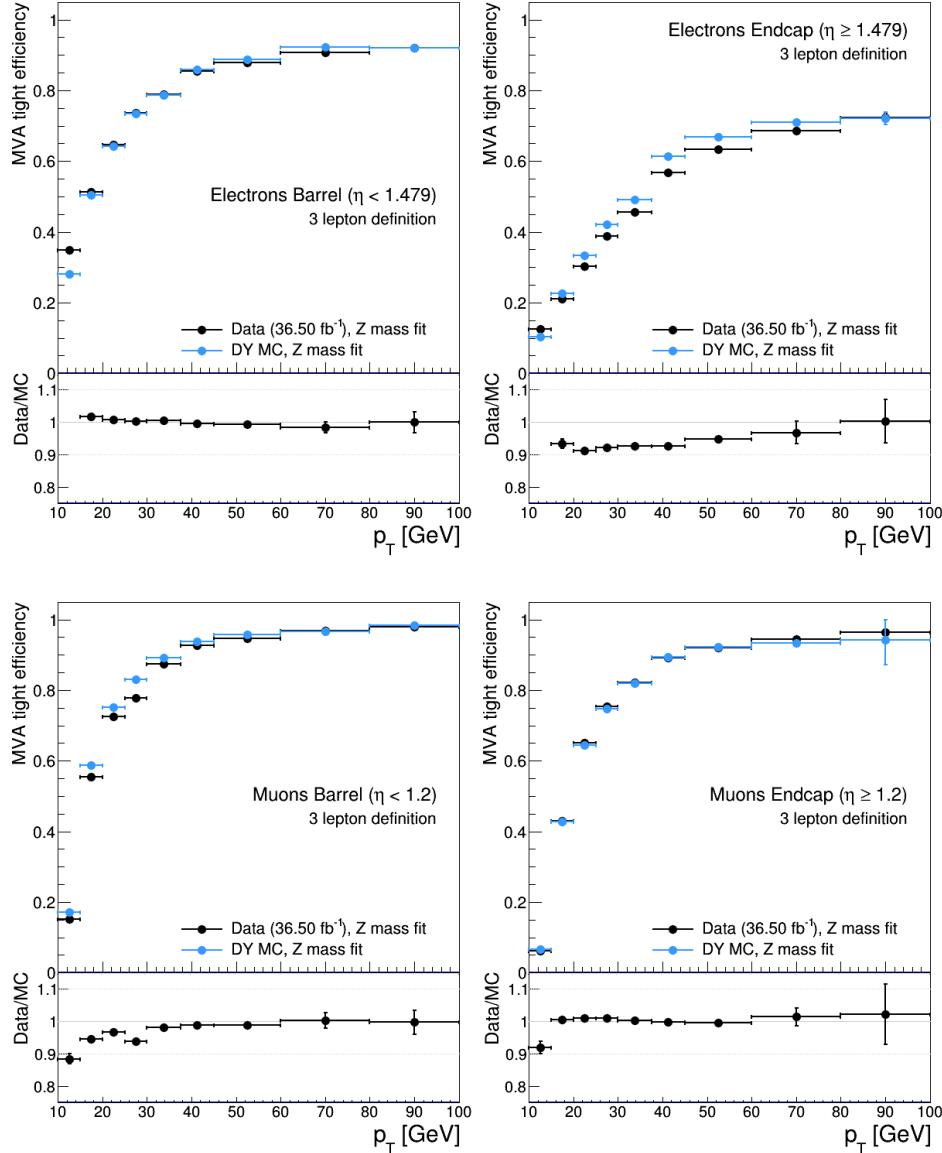


Figure 6.9: Tight vs loose selection efficiencies for electrons (top), and muons (bottom), for the 3l channel not including the tight-charge requirement.

2653 full sample; therefore, the full simulation correction is given by the product of all
 2654 the individual scale factors. The scale factors used in this thesis are inherited from
 2655 Reference [149] which in turns inherited them from leptonic SUSY analyses using
 2656 equivalent lepton selections.

2657 The efficiency of applying the tight selection as defined in Tables 6.4 and 6.5, on the
 2658 loose leptons are determined by using a tag and probe method on a sample of Drell-
 2659 Yan enriched events. Figures 6.8 and 6.9 show the efficiencies for the $2lss$ channel and
 2660 $3l$ channel respectively. Efficiencies in the $2lss$ channel have been produced including
 2661 the tight-charge requirement, while for the $3l$ channel it is not included. Number
 2662 of passed and failed probes are determined from a fit to the invariant mass of the
 2663 dilepton system. Simulation is corrected using these scale factors; note that they
 2664 depends on η and p_T .

2665 6.5.3 Jets and b -jet tagging

2666 In this analysis, jets are reconstructed by clustering PF candidates using the anti- k_t
 2667 algorithm with parameter distance $\Delta R = 0.4$; those charged hadrons that are not
 2668 consistent with the selected primary vertex are discarded from the clustering. The
 2669 jet energy is then corrected for the varying response of the detector as a function
 2670 of transverse momentum p_T and pseudorapidity η . Jets are selected for use in the
 2671 analysis only if they have $p_T > 25$ GeV and are separated from any selected leptons
 2672 by $\Delta R > 0.4$.

2673 Jets coming from the primary vertex and jets coming from pile-up vertices are
 2674 distinguished using a MVA discriminator based on the differences in the jet shapes,
 2675 in the relative multiplicity of charged and neutral components, and in the different
 2676 fraction of transverse momentum which is carried by the most energetic components.

2677 Jet tracks are also required to be compatible with the primary vertex.

2678 Jets originated from the hadronization of a b quark are selected using a MVA
 2679 likelihood discriminant which uses track-based lifetime information and reconstructed
 2680 secondary vertices (CSV algorithm). Only jets within the CMS tracker acceptance
 2681 ($\eta < 2.4$) are identified with this tool. Data samples are used to measure the efficiency
 2682 of the b -jet tagging and the probability to misidentify jets from light quarks or gluons;
 2683 in both cases the measurements are parametrized as a function of the jet p_T and η
 2684 and later used to correct differences between the data and MC simulation in the b
 2685 tagging performance, by applying per-jet weights to the simulation, dependent on
 2686 the jet p_T , η , b tagging discriminator, and flavor (from the MC generation/simulation
 2687 truth information) [151]. The per-event weight is taken as the product of the per-jet
 2688 weights, including those of the jets associated to the leptons. The weights are derived
 2689 on $t\bar{t}$ and Z+jets events.

2690 Two working points are defined, based on the CSV algorithm output: *loose* work-
 2691 ing point ($\text{CSV} > 0.46$) with a b signal tagging efficiency of about 83%, and *medium*
 2692 working point ($\text{CSV} > 0.80$) with b -tagging efficiency of about 69% [152]. Tagging of
 2693 jets from charm quarks have efficiencies of about 40% and 18% for loose and medium
 2694 working points respectively. Separate scale factors are applied to jets originating from
 2695 bottom/charm quarks and from light quarks in simulated events to match the tagging
 2696 efficiencies measured in the data.

2697 6.5.4 Missing Energy MET

2698 As stated in Section 3.4.1, the MET vector is calculated as the negative of the vector
 2699 sum of transverse momenta of all PF candidates in the event and its magnitude is
 2700 referred to as E_T^{miss} . Due to pile-up interactions, the performance in determining

2701 MET is degraded; in order to correct for that, the energy from the selected jets and
 2702 leptons that compose the event is assigned to the variable H_T^{miss} . It is calculated in
 2703 the same way as E_T^{miss} and although it has worse resolution than E_T^{miss} , it is more
 2704 robust in the sense that it does not rely on the soft part of the event. The event
 2705 selection uses a linear discriminator based on the two variables given by

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

2706 taking advantage of the fact that the correlation between E_T^{miss} and H_T^{miss} is less
 2707 for events with instrumental missing energy than for events with real missing energy.
 2708 The working point $E_T^{miss, LD} > 0.2$ was chosen to ensure a good signal efficiency while
 2709 keeping an efficient background rejection.

2710 6.6 Event selection

2711 Events are selected considering the features of the signal process and the decay sig-
 2712 nature as described in Section 6.2. At the trigger level, events are selected to contain
 2713 either one, two, or three leptons with minimal p_T thresholds:

- 2714 • single-lepton trigger → 24 GeV for muons and at 27 GeV for electrons
- 2715 • double-lepton triggers → leading and sub-leading leptons: 17 and 8 GeV for
 2716 muons and 23 and 12 GeV for electrons.
- 2717 • three-lepton triggers → threshold on the third hardest lepton in the event: 5
 2718 and 9 GeV for muons and electrons, respectively.

2719 The offline event selection level targets the specific topology of the tHq signal
 2720 with $H \rightarrow WW$ and $t \rightarrow Wb \rightarrow l\nu b$; therefore, the resulting state is composed of three

2721 W bosons, one b quark, and a light spectator quark at high rapidity. The selection
 2722 criteria for the two channels exploited in this analysis are summarized in Table 6.6.
 2723 This selection includes contributions from $H \rightarrow \tau\tau$ and $H \rightarrow ZZ$ as well.

Same-sign $\ell\ell$ channel $e^\pm\mu^\pm, \mu^\pm\mu^\pm$	$\ell\ell\ell$ channel
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.

2724 In the $2lss$ channel, events with additional tight leptons are vetoed as well as those
 2725 for which a loose lepton pair has an invariant mass below 12 GeV. A threshold in p_T of
 2726 the leading and sub-leading leptons is also required. Events where the two electrons
 2727 have invariant mass within 10 GeV of the Z boson mass (Z -veto) are discarded in
 2728 order to reject events from DY+jets production with charge misidentified electrons.

2729 In addition, contribution from the associated production of two W bosons of equal
 2730 charge and two light jets $W^\pm W^\pm qq$ and from same-sign W boson pairs can also be
 2731 produced in double parton scattering (DPS) processes, where each of the colliding
 2732 protons gives two partons, resulting in two hard interactions.

2733 In the $3l$ lepton channel, leptons are required to have respectively $p_T > 25\text{GeV}, >$
 2734 $> 15\text{ GeV}$, and $> 15\text{ GeV}$. Events with an opposite-sign same-flavor lepton combination
 2735 (OSSF) with invariant mass within 15 GeV of the Z boson mass are discarded in order
 2736 to reject events from $WZ + \text{jets}$ production.

2737 6.7 Background modeling and predictions

2738 The dominant background contribution is expected to arise from top quark produc-
2739 tion processes, either $t\bar{t}$ pair production or in $t\bar{t}$ associated production with a W/Z.
2740 Processes with production of single top quarks also contribute, mainly in the associ-
2741 ated production with a Z boson (tZq) or when produced with both a W and a Z boson
2742 (tZW). Background contamination from diboson processes is strongly suppressed by
2743 imposing the Z-veto, vetoing additional leptons and requiring b -jets in the event.

2744 The selection criteria in Table 6.6 represent a relatively loose selection that allows
2745 to maintain a large signal efficiency while suppressing the main backgrounds; thus
2746 that selection is called *pre-selection*. The events obtained from the pre-selection are
2747 then used to extract the signal contribution in a second analysis step, using BDT dis-
2748 criminators against the main backgrounds of $t\bar{t}W/t\bar{t}Z$ and non-prompt leptons from
2749 $t\bar{t}$. The shape of the discriminator variables is then fit to the observed data distribu-
2750 tion to estimate the signal and background yields, simultaneously for all channels.

2751 Irreducible backgrounds are reliably estimated from MC simulated events; there-
2752 fore, in this analysis all backgrounds involving prompt leptons are estimated in this
2753 way. Reducible backgrounds, like non-prompt lepton backgrounds, are not well pre-
2754 dicted by simulation, hence, they are estimated using data-driven methods.

2755 6.7.1 $t\bar{t}V$ and diboson backgrounds

2756 Backgrounds from $t\bar{t}W$ and $t\bar{t}Z$ processes are estimated using simulated events, cor-
2757 rected for data/MC differences and inefficiencies (trigger and lepton selection) in the
2758 same way as signal events. Their production cross sections are calculated at NLO of
2759 QCD and EWK, considering theoretical uncertainties from unknown higher orders of
2760 12% for $t\bar{t}W$ and 10% for $t\bar{t}Z$. Additional uncertainties arise from the knowledge of

2761 PDFs and α_s of about 4% each for $t\bar{t}W$ and $t\bar{t}Z$.

2762 The diboson contribution is also estimated from simulated events; however, the
 2763 overall normalization of this process is obtained from a dedicated control region.
 2764 The motivation behind that strategy is that even though the measured inclusive
 2765 cross section for diboson processes (WZ, ZZ) is in good agreement with the NLO
 2766 calculations [149], that agreement is perturbed when leptonic Z decays and hadronic
 2767 jets in the final state are required; those requirements are precisely the ones that
 2768 make the diboson production a background for the tHq signal. Thus, by using a
 2769 dedicated control region dominated by WZ production⁴, the overall normalization is
 2770 constrained.

2771 The control region is defined by the presence of at least three leptons, of which
 2772 one opposite-sign pair must be compatible with a Z boson decay, i.e., invert the Z -
 2773 veto which makes the control region orthogonal to signal region; the b-jet tagging
 2774 requirements is also inverted with respect to the signal region, i.e., require two not
 2775 b -jets. A scale factor is extracted from the predicted distribution of WZ events in the
 2776 control region, and the observed data, while keeping other processes fixed; this factor
 2777 is used to scale the diboson prediction in the signal selection region. More details
 2778 about the procedure used can be found in Reference [149] from where the scale factor
 2779 is taken.

2780 In order to test the usability of the diboson background scale factor in this analysis,
 2781 a Z -enriched control region⁵ was defined by inverting the Z -veto and requiring exactly
 2782 three tight leptons with $p_T > 25/15/15$ GeV, one or more jets passing the CSVv2 loose
 2783 working point and less than four central jets. Figure 6.10 shows the distribution of
 2784 three variables in the diboson control region; the good agreement between MC and

⁴ ZZ background is strongly reduced by the cut on MET.

⁵ This control region is different to the one used to find the scale factor.

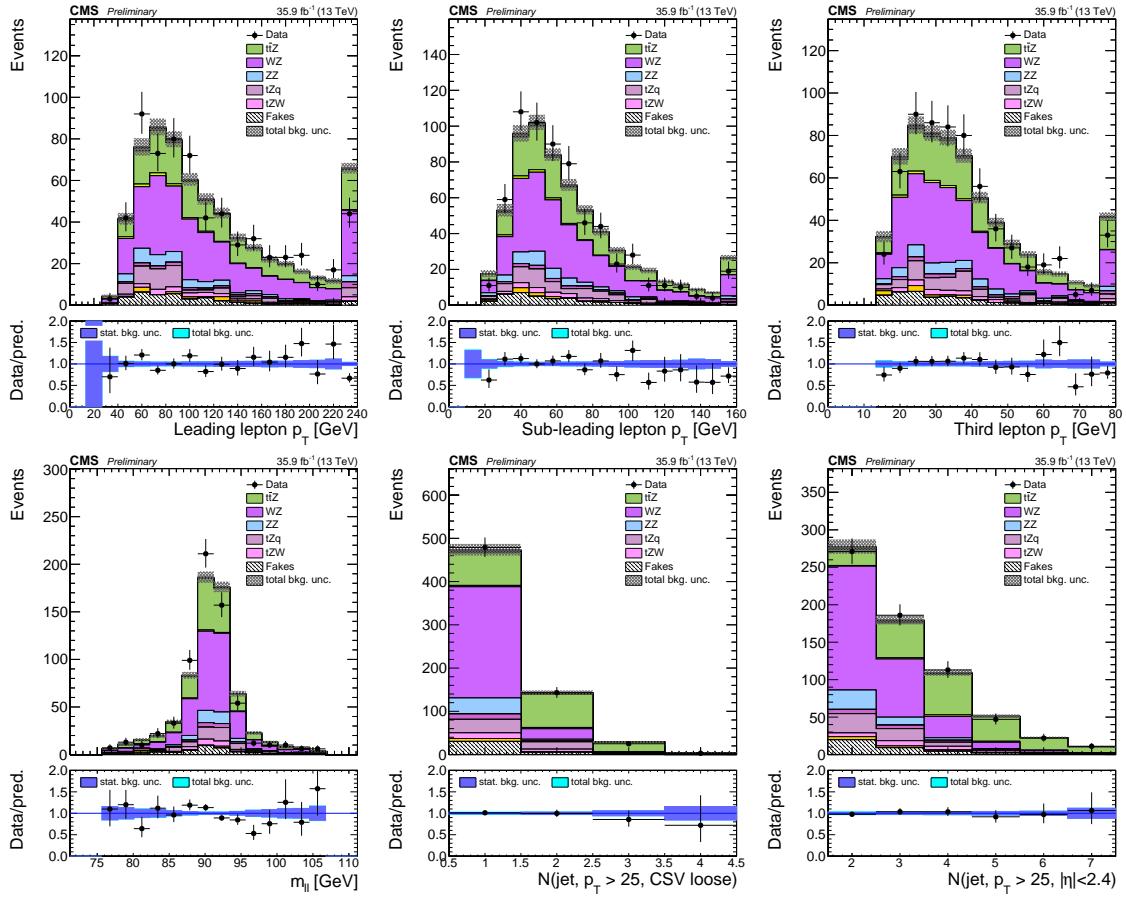


Figure 6.10: Kinematic distributions in the diboson control region.

2785 data motivates the adoption of the diboson background scale factor.

2786 Most of the diboson events passing the signal selection contain jets from light
 2787 quarks and gluons that are incorrectly tagged as b -jets; it makes the estimate mainly
 2788 sensitive to the experimental uncertainty in the mis-tag rate rather than the theore-
 2789 tical uncertainty in the jet flavor composition. The overall uncertainty assigned to
 2790 the diboson prediction is estimated from the statistical uncertainty due to the limited
 2791 sample size in the control region (30%), the residual background in the control region
 2792 (20%), the uncertainties on the b -tagging rate (10-40%), and from the knowledge of
 2793 PDFs and the theoretical uncertainties of the extrapolation (up to 10%).

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

²⁷⁹⁵ The non-prompt lepton background contribution to the final selection is estimated
²⁷⁹⁶ using the fake factor method. The main idea of the method is to define a control
²⁷⁹⁷ region of events enriched in the background to estimate and determine a factor that
²⁷⁹⁸ relates (extrapolates) these events to those in the signal region. The method is data-
²⁷⁹⁹ driven in the sense that the control sample is selected from data, and the extrapolation
²⁸⁰⁰ factor is measured from data.

²⁸⁰¹ In the signal region of this analysis, non-prompt leptons are predominantly pro-
²⁸⁰² duced in $t\bar{t}$ events, with a much smaller contribution, from Drell-Yan production;
²⁸⁰³ therefore, the control region also know as *application region*, is defined by modifying
²⁸⁰⁴ the event selection criteria in such a way that most of the events after selection are
²⁸⁰⁵ $t\bar{t}$ events and thus the misidentification rate is increased. The application regions
²⁸⁰⁶ for electrons and muons are defined by the fakeable object definitions in Tables 6.4
²⁸⁰⁷ and 6.5. Since the fakeable definition is a loosened version of the tight definition, in
²⁸⁰⁸ the context of fake rates the fakeable definition becomes the loose selection.

²⁸⁰⁹ The ratio between the number of events that pass both, the loose and tight se-
²⁸¹⁰ lections, and the number of events that pass the loose selection but fail the tight
²⁸¹¹ one, corresponds to the *loose-to-tight ratio or fake factor/rate (f)*. The measurement
²⁸¹² of the fake factor is made using two background dominated data samples, collected
²⁸¹³ with dedicated triggers, as a function of p_T and $|\eta|$ and separately for muons and
²⁸¹⁴ electrons:

- ²⁸¹⁵ • A sample dominated by QCD multijet events, collected using single lepton trig-
²⁸¹⁶ gers at relatively high p_T thresholds. It is used to extract ratios for lepton
²⁸¹⁷ candidates with p_T above 30 GeV.
- ²⁸¹⁸ • A sample dominated by Z + jets events, where the two high p_T leptons resulting

2819 from the Z decay are used to trigger the events without biasing the p_T spectrum
 2820 of a third lepton at low transverse momentum. It is used to determine the ratios
 2821 for low p_T leptons.

2822 Processes like $W + \text{jets}$, $Z + \text{jets}$, WZ and ZZ produce prompt leptons that
 2823 contaminate the samples; thus, they are suppressed by vetoing additional leptons in
 2824 the selection, and the residual contamination is then subtracted using the transverse
 2825 mass as a discriminating variable.

2826 The extrapolation from the application region to the signal region is performed
 2827 by weighting the events in the application region using the fake factor according to
 2828 the following rules:

2829 • events with one lepton failing the tight criteria are weighted with the factor
 2830 $\frac{f}{(1-f)}$ for the estimate to the signal region.

2831 • events with two leptons (i,j) failing the tight criteria are weighted with the factor
 2832 $-\frac{f_i f_j}{(1-f_i)(1-f_j)}$ for the estimate to the signal region.

2833 • events with three leptons (i,j,k) failing the tight criteria are weighted with the
 2834 factor $\frac{f_i f_j f_k}{(1-f_i)(1-f_j)(1-f_k)}$ for the estimate to the signal region.

2835 Figure 6.11 shows the fake rates for electrons and muons used in this analysis
 2836 which were taken from the studies in Reference [149].

2837 The resulting prediction of the event yield in the signal selection carries an uncer-
 2838 tainty of 30-50% which is composed of the statistical uncertainty in the measurement
 2839 of the fake rates due to prescaling of lepton triggers, the uncertainty in the subtraction
 2840 of residual prompt leptons from the control region, and from testing the closure of the
 2841 method in simulated background events; hence, it is one of the dominant limitations
 2842 on the performance of multilepton analyses in general and this analysis in particular.

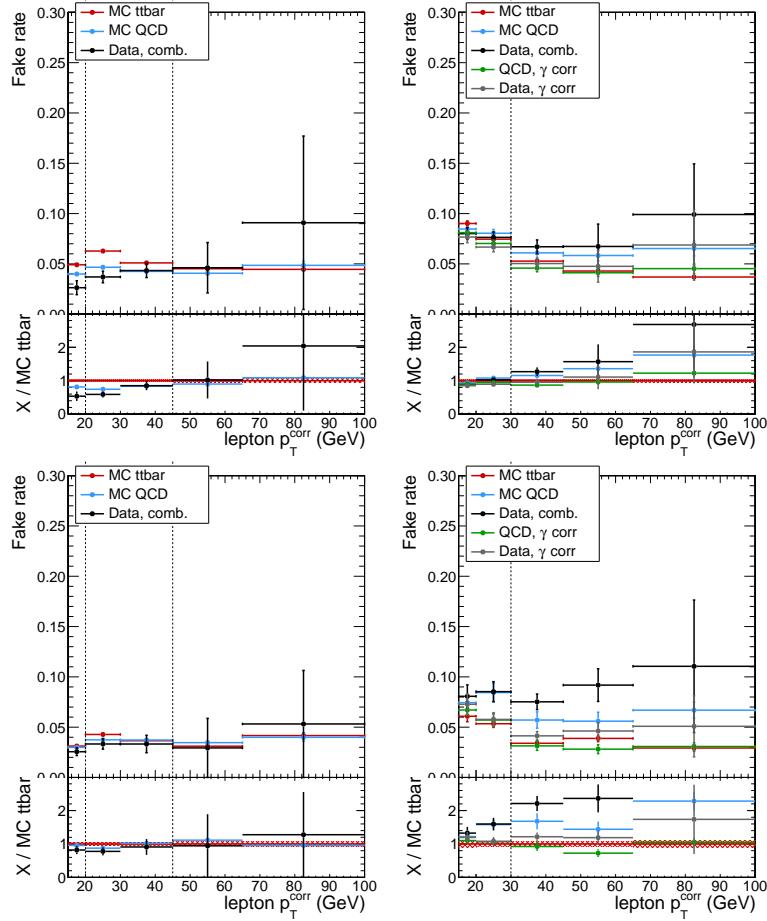


Figure 6.11: Fake rate measurement in events in data for muons (left column) and electrons (right column). Predictions from simulated events in the measurement region (blue) and from non-prompt leptons in $t\bar{t}$ (red) are included for comparison. Top row is for $|\eta| < 2.5$ and bottom row for $|\eta|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

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 η ,

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 ± 0.0011	0.0179 ± 0.0004	0.0262 ± 0.0020
$1.48 \leq \eta < 2.5$	0.1329 ± 0.0066	0.1898 ± 0.0014	0.3067 ± 0.0113
MC			
$0 \leq \eta < 1.48$	0.0378 ± 0.0016	0.0222 ± 0.0003	0.0233 ± 0.0015
$1.48 \leq \eta < 2.5$	0.0956 ± 0.0044	0.2108 ± 0.0027	0.3157 ± 0.0018

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

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

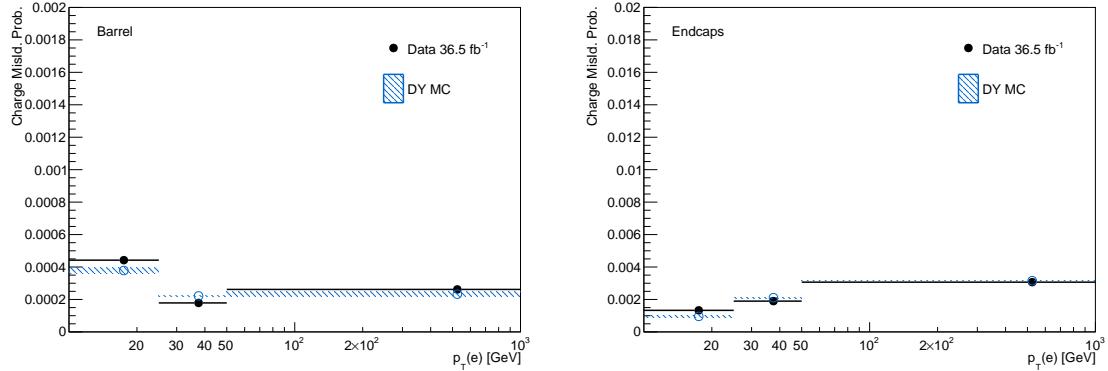


Figure 6.12: Electron charge mis-ID probabilities as a function of p_T for $|\eta| < 2.5$ (left) and $|\eta| < 2.5$ (right) [149].

The contribution from charge mis-ID electrons in signal selection of this analysis comes mainly from $t\bar{t}$ and Drell-Yan events. The systematic uncertainty of the normalization of the charge mis-id. estimate is evaluated at about 30%, arising from a slight disagreement of the mis-ID. probability between data and simulation. Given that it only affects the $e\mu$ channel, its impact on the final sensitivity is very limited.

2861 6.8 Pre-selection yields

2862 The expected and observed event yields of the pre-selection are shown in Table 6.8;
 2863 Figure 6.13 shows the distributions of some relevant kinematic variables, normalized
 2864 to the cross section of the respective processes and to the integrated luminosity. The
 2865 remaining variables distributions are shown in Appendix B.1.

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

2866 For the tH and $t\bar{t}H$ processes, the largest contribution comes from Higgs decays
 2867 to WW (about 75%), followed by $\tau\tau$ (about 20%) and ZZ (about 5%). Other Higgs
 2868 production modes contribute negligible event yields (< 5% of the $tH+t\bar{t}H$ yield) as
 2869 shown in Table 6.9.

2870 A significant fraction of selected data events (about 50% in the dilepton channels,
 2871 and about 80% in the trilepton channel) also passes the selection used in the dedicated

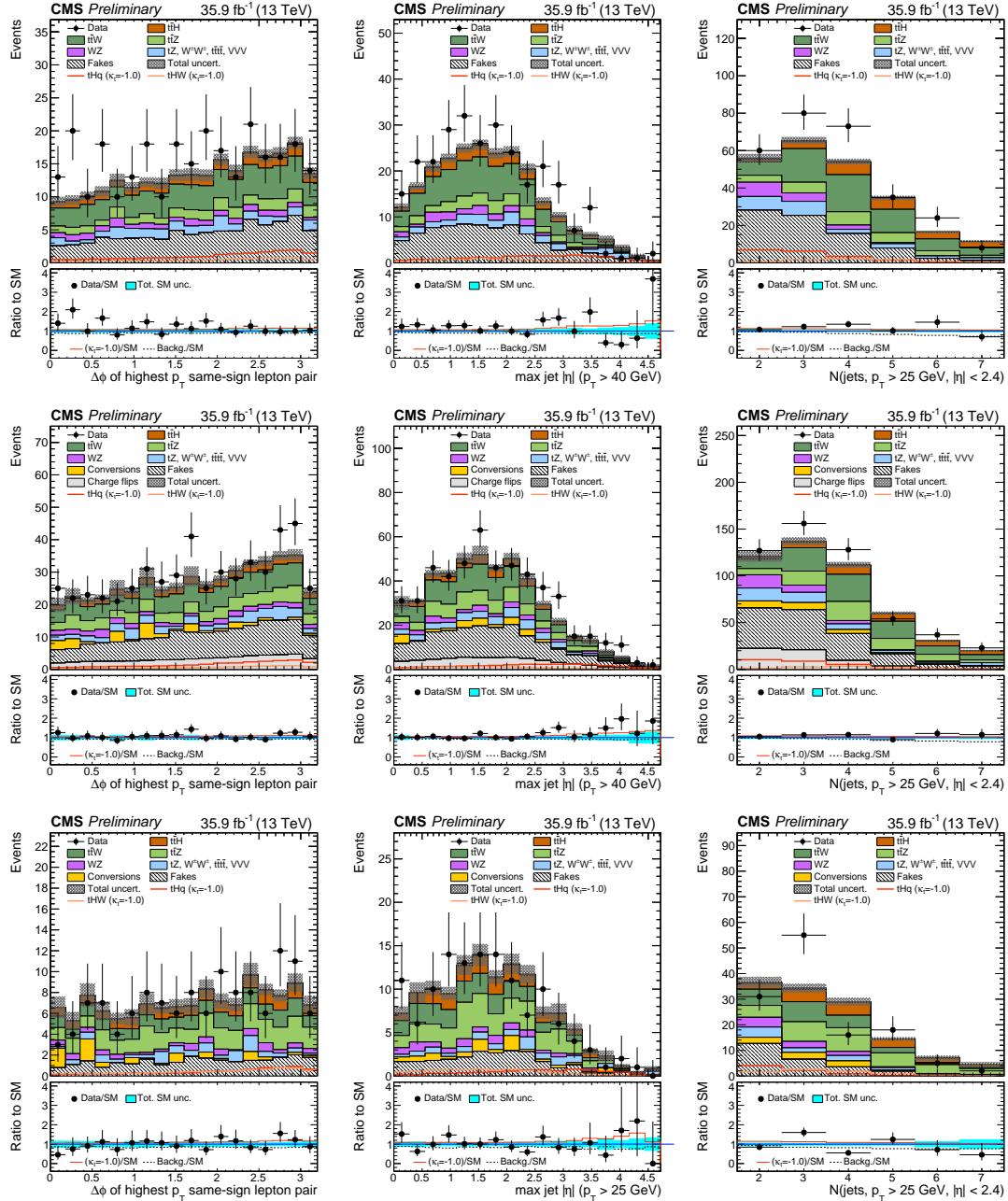


Figure 6.13: Distributions of discriminating variables for the event pre-selection for the same-sign $\mu^{\pm}\mu^{\pm}$ channel (top row), the same-sign $e^{\pm}\mu^{\pm}$ channel (middle row) and three lepton channel (bottom row), normalized to 35.9 fb^{-1} , before fitting the signal discriminant 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 $\kappa_t = -1.0, \kappa_V = 1.0$.

	3ℓ	$\mu^\pm \mu^\pm$	
tHq (Inclusive)	6.57	100.0%	17.38 100.0%
$tHq(H \rightarrow WW)$	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)	7.32	100.0%	7.62 100.0%
$tHW(H \rightarrow WW)$	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.

2872 search for tH in multilepton channels [149]. This is particularly important when
 2873 considering a possible combination of the measurements from both studies. More
 2874 details about the overlap between this both analyses are presented in Appendix E.

2875 6.9 Signal discrimination

2876 The production cross section for the signal processes tHq , tHW , and $t\bar{t}H$ is only
 2877 about 600 fb (the enhancement provided by inverted couplings, $\kappa_t = -1$ almost double
 2878 it), resulting in a small signal to background ratio even for a tight selection. A
 2879 multivariate method is hence employed to train discriminators to separate tH signal
 2880 events from the dominant background events.

2881 **6.9.1 MVA classifiers evaluation**

2882 Several MVA classifier algorithms were evaluated in order to determine the most
 2883 appropriate method for this analysis⁶. The comparison is based on the performance
 2884 of the classifiers, encoded in the plot of the background rejection as a function of the
 2885 signal efficiency (ROC curve). The top row of Figure 6.14 shows the ROC curves
 2886 for the several methods evaluated; two separated training were performed in the $3l$
 2887 channel: against $t\bar{t}$ (right) and $t\bar{t}V$ (left) processes.

2888 In both cases, the gradient boosted decision tree *BDTG* (*BDTA_GRAD* in the
 2889 plot) classifier offers the best results, followed by the adaptive BDT classifier (*BDTA*);
 2890 the several Fisher classifiers tested, which differ in their parameters and/or boosting
 2891 method, they offer similar performance among them, while the k-Nearest Neighbour
 2892 (kNN) classifier performance is below the rest of the classifiers. The corresponding
 2893 ROC curves and in the $2lss$ channel for trainings against $t\bar{t}V$ (left) and $t\bar{t}$ (right)
 2894 processes are shown in the bottom row of Figure 6.14; the BDTG performance is
 2895 similar to that in the $3l$ channel.

2896 **6.9.2 Discriminating variables**

2897 The classifier chosen to separate the tHq signal from the main backgrounds is the
 2898 *BDTG* classifier, trained on simulated signal and background events. The samples
 2899 used in the training are the tHq sample in Table 6.2, the samples in the third section
 2900 of table A.4 and the samples marked with an * in the same table.

2901 As explained in Section 5.1.1, a set of discriminating variables are given as input to
 2902 the *BDTG* which combines the individual discrimination power of each input variable

⁶ 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]

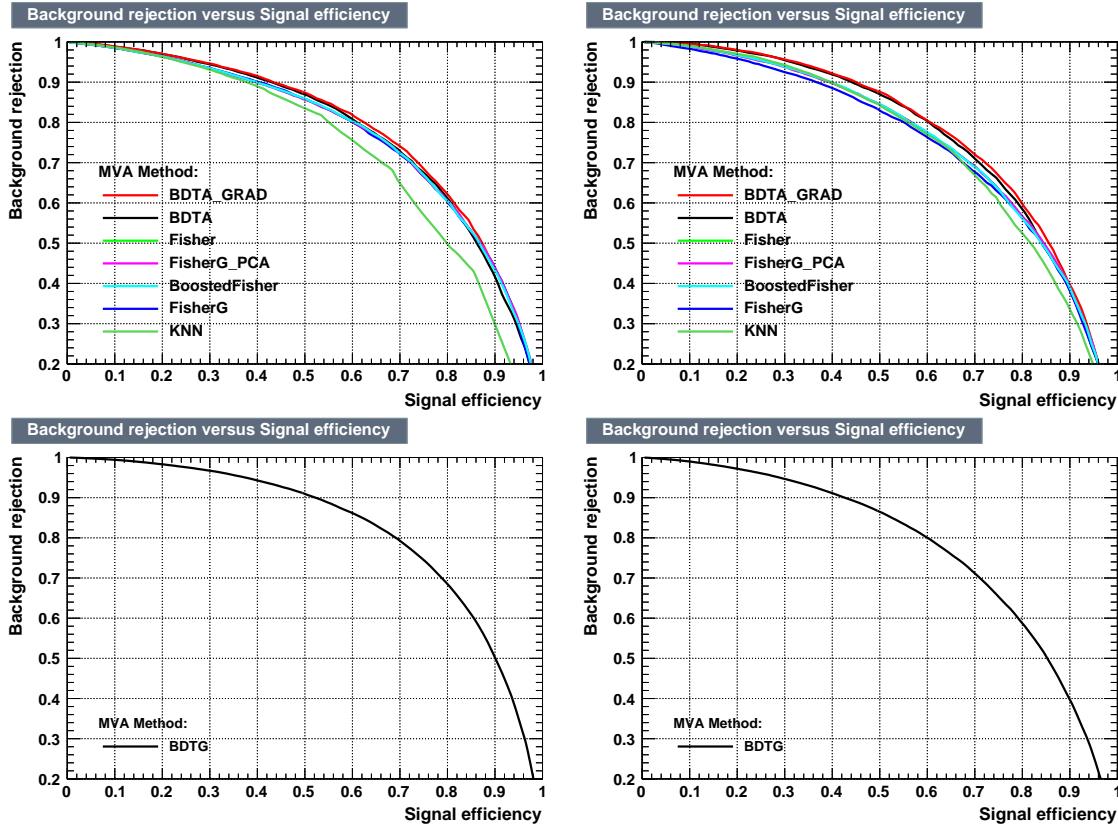


Figure 6.14: Top: Background rejection vs signal efficiency (ROC curves) for various MVA classifiers in the $3l$ channel for training against $t\bar{V}$ (left) and $t\bar{t}$ (right). Bottom: background rejection vs signal efficiency (ROC curve) in the $2lss$ channel for a single discriminator: BDTG, against $t\bar{V}$ (left) and $t\bar{t}$ (right).

2903 to produce a discriminator with the maximum discrimination power. Table 6.10 lists
 2904 the input variables used in the BDTG trainings for this analysis. The same set of
 2905 input variables was used to produce the plots for MVA classifiers evaluation.

2906 Plots in Figure 6.15 shows the BDTG input variables distributions for the signal
 2907 and background samples, in the $3l$ channels.

2908 All the input variables have some discrimination power, however, that power is
 2909 bigger for some of them; for instance, the third lepton p_T plot (top left in Figure 6.15)
 2910 shows some discrimination power against WZ and VVV backgrounds for which there
 2911 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 rd lepton (2 nd for ss2l)
totCharge	Sum of lepton charges
minDRll	Min ΔR 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.

2912 power does not cover all the backgrounds, it counts for the final discriminator. A
 2913 similar situation can be seen in the plot for the number of jets (row three, column two);
 2914 $t\bar{t}W$, $t\bar{t}Z$ and $t\bar{t}H$ processes tend to have more jets compared to the tHq process. The
 2915 discrimination power is more evident in other plots like in the plot of the maximum
 2916 $|\eta|$ of the jets in the event (row two, column three). The same or equivalent input
 2917 variables are found to be performing well for both $3l$ and $2lss$ channels. Figure B.4
 2918 shows the corresponding input variables distribution plots for the $2lss$ channel.

2919 **Discrimination power from BDTG classifier**

2920 The Discrimination power of the input variables can also be evaluated from the BDTG
 2921 training, exclusively for the training samples, i.e., dominant backgrounds ($t\bar{t}$ and $t\bar{t}V$);
 2922 the training samples are submitted to the selection cuts on Table 6.6.

2923 Figure 6.16 shows the comparison between input variables for the two trainings
 2924 in the $3l$ channel; it reveals that some variables show opposite behavior for the two
 2925 background sources, which results in potentially screening the discrimination power
 2926 if they were to be used in a single discriminant, i.e., if the training would join $t\bar{t}$ and

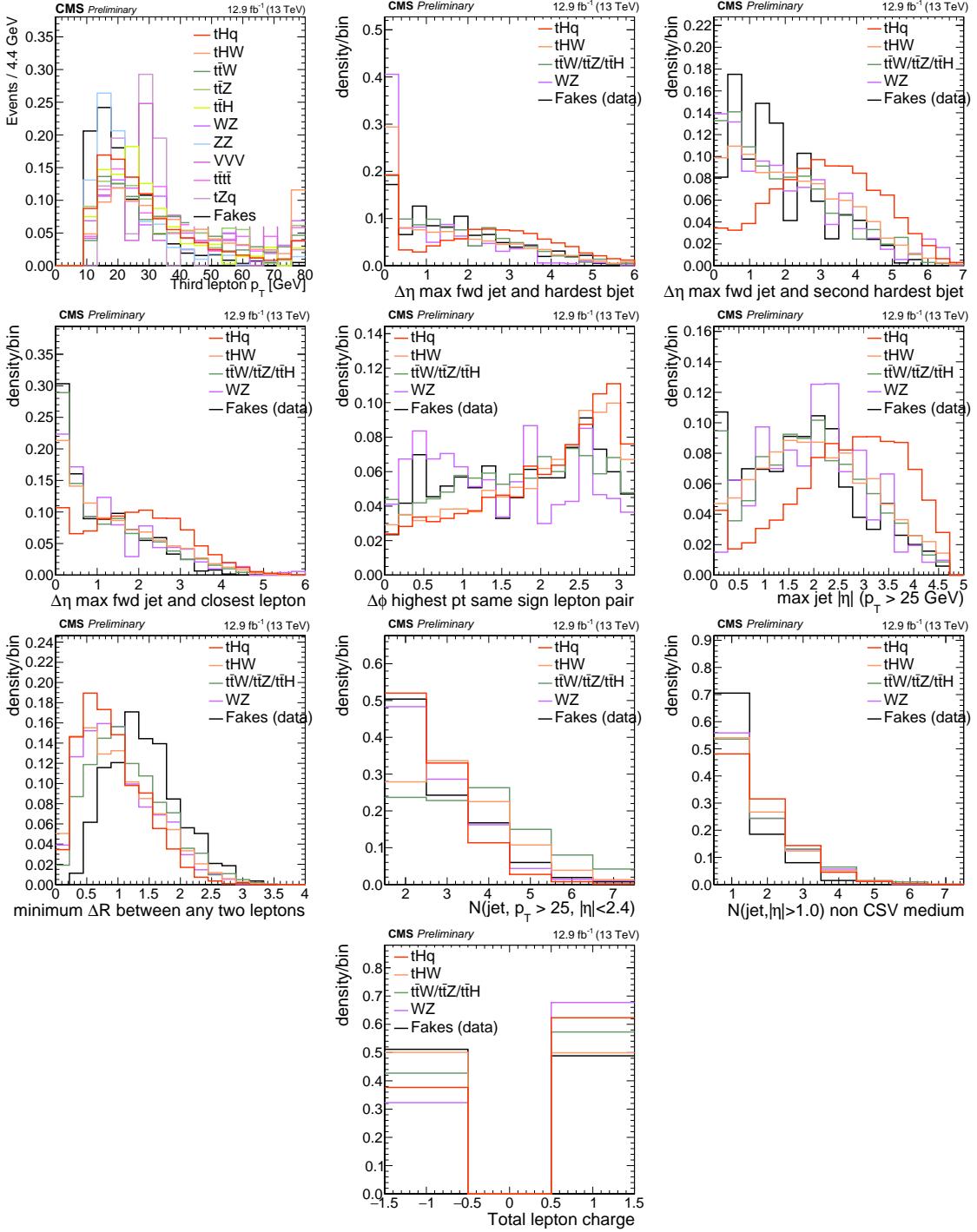


Figure 6.15: Distributions of the BDTG classifier input variables (not normalized) for signal discrimination in the $3l$ channel.

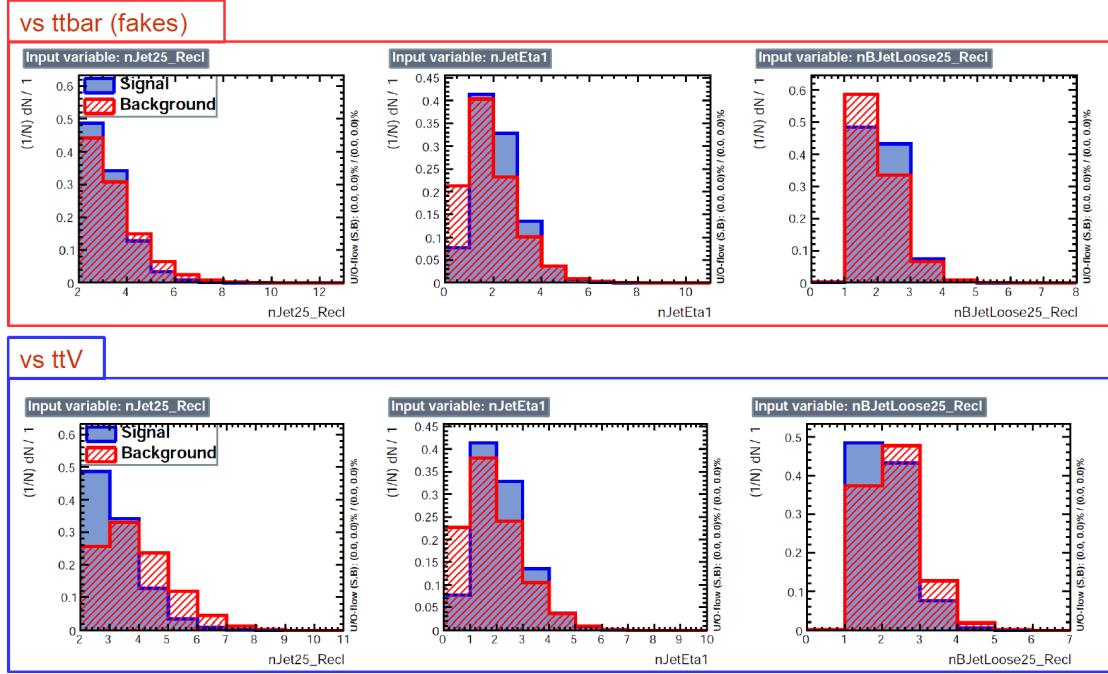


Figure 6.16: BDT input variables as seen by BDTG classifier for the $3l$ channel, tHq signal(blue) discriminated against ttV background (red).

2927 $tt\bar{V}$. For some other variables the distributions are similar in both background cases.

2928 In contrast to the distributions in Figure 6.15 only the dominant backgrounds are
2929 included; however, the discrimination power agrees among plots.

2930 Figures in the Appendix B.5, B.6, B.7, and B.8 show the input variables
2931 distributions for the $2lss$ and $3l$ channel as seen by the BDTG classifier.

2932 Input variables correlations

2933 From Table 6.10, it is clear that the input variables are correlated to some extent.
2934 These correlations play an important role for some MVA methods like the Fisher
2935 discriminant method in which the first step consist of performing a linear transfor-
2936 mation to an phase space where the correlations between variables are removed. In
2937 the case of BDT, correlations do not affect the performance. Figure 6.17 shows the

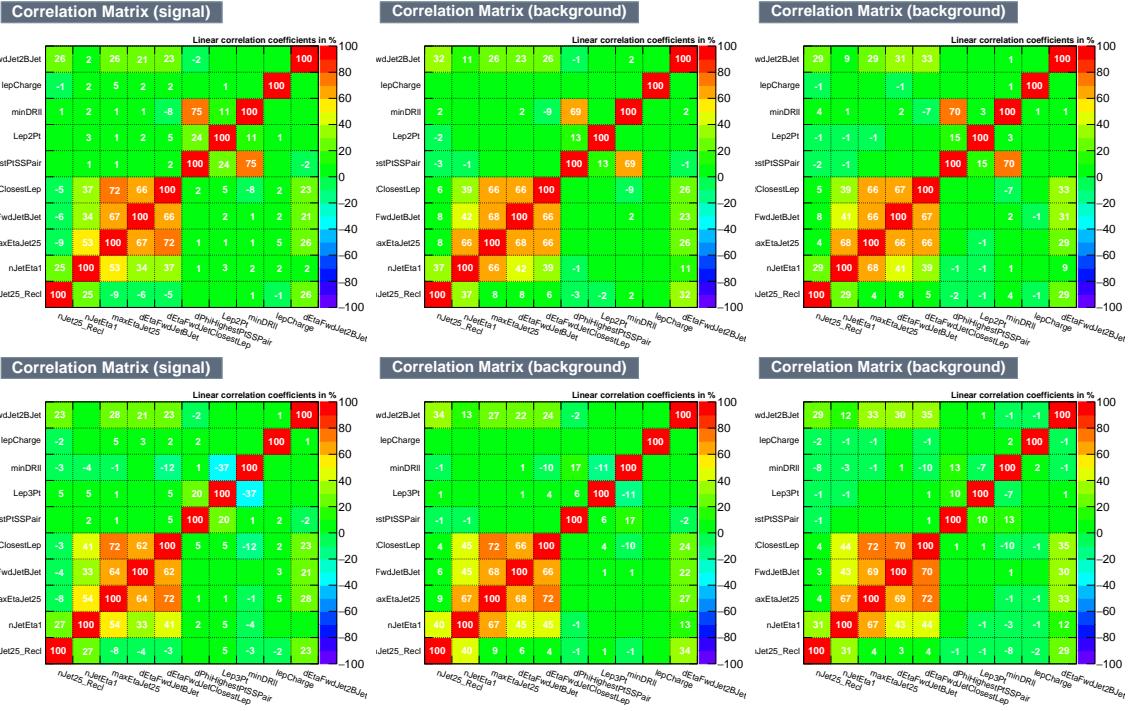


Figure 6.17: Signal (left), $t\bar{t}$ background (middle), and $t\bar{t}V$ background (right.) correlation matrices for the input variables in the BDTG classifier for the $2lss$ (top) and $3l$ (bottom) channels.

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

6.9.3 BDTG classifiers response

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

In order to explore further optimization in the BDTG performance, several changes

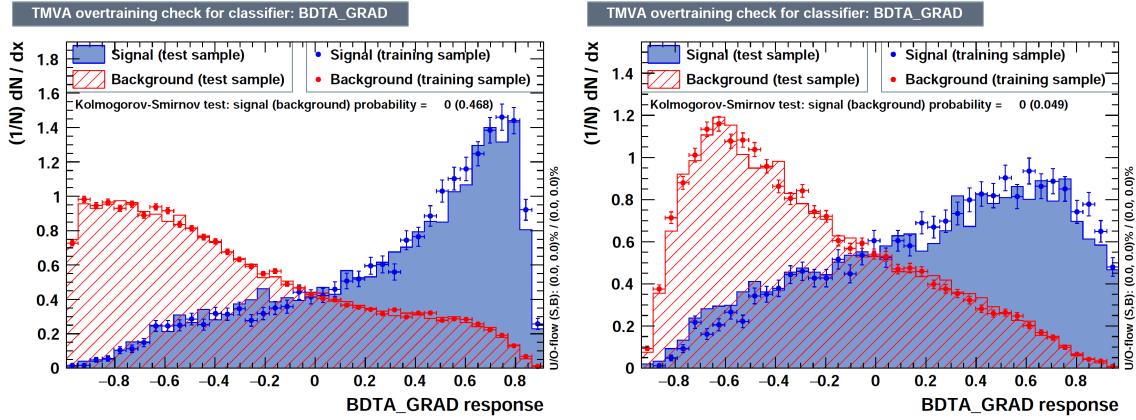


Figure 6.18: BDTG classifier output for trainings against $t\bar{t}V$ (left) and $t\bar{t}$ (right). Default BDTG parameters have been used.

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 jet

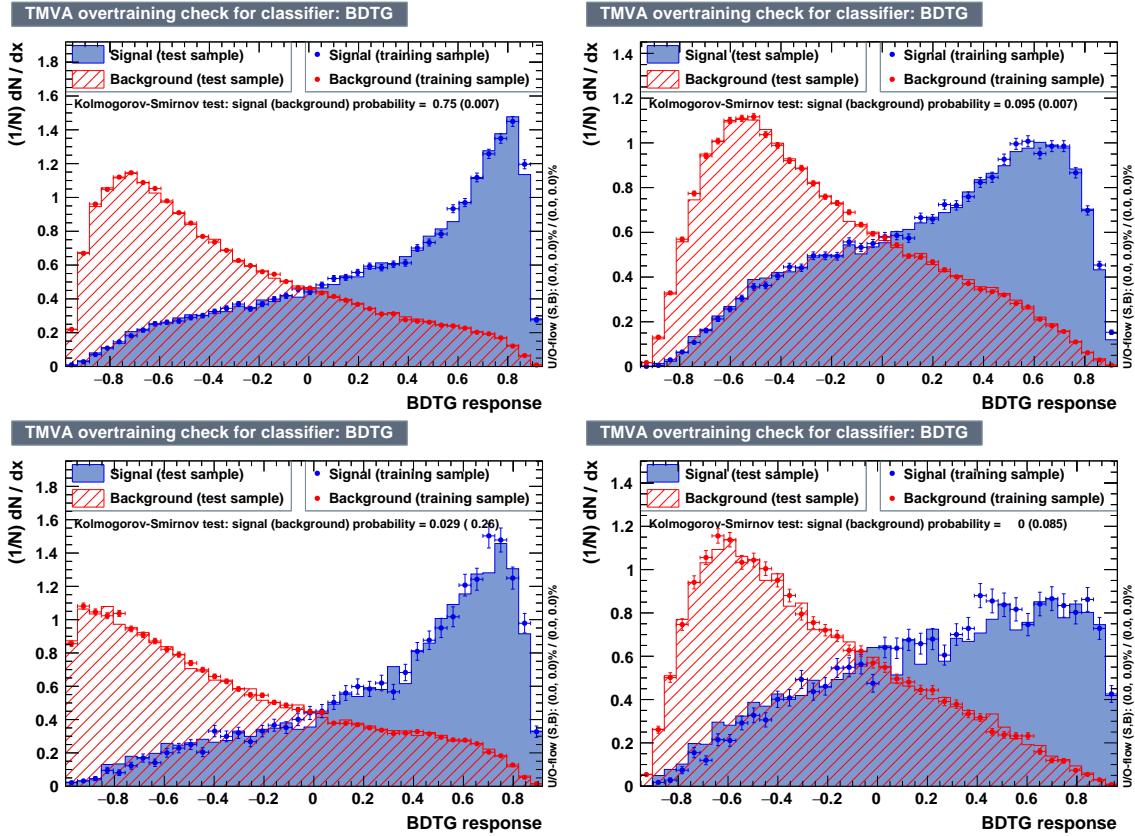


Figure 6.19: BDTG classifiers output for training against $t\bar{V}$ (left) and $t\bar{t}$ (right) for $2lss$ channel(top) and $3l$ channel (bottom) .

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

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

2967 The improvement in the discrimination performance provided by the additional
 2968 variables is about 1%, so it was decided not to include them in the procedure. Table
 2969 6.13 show 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% .

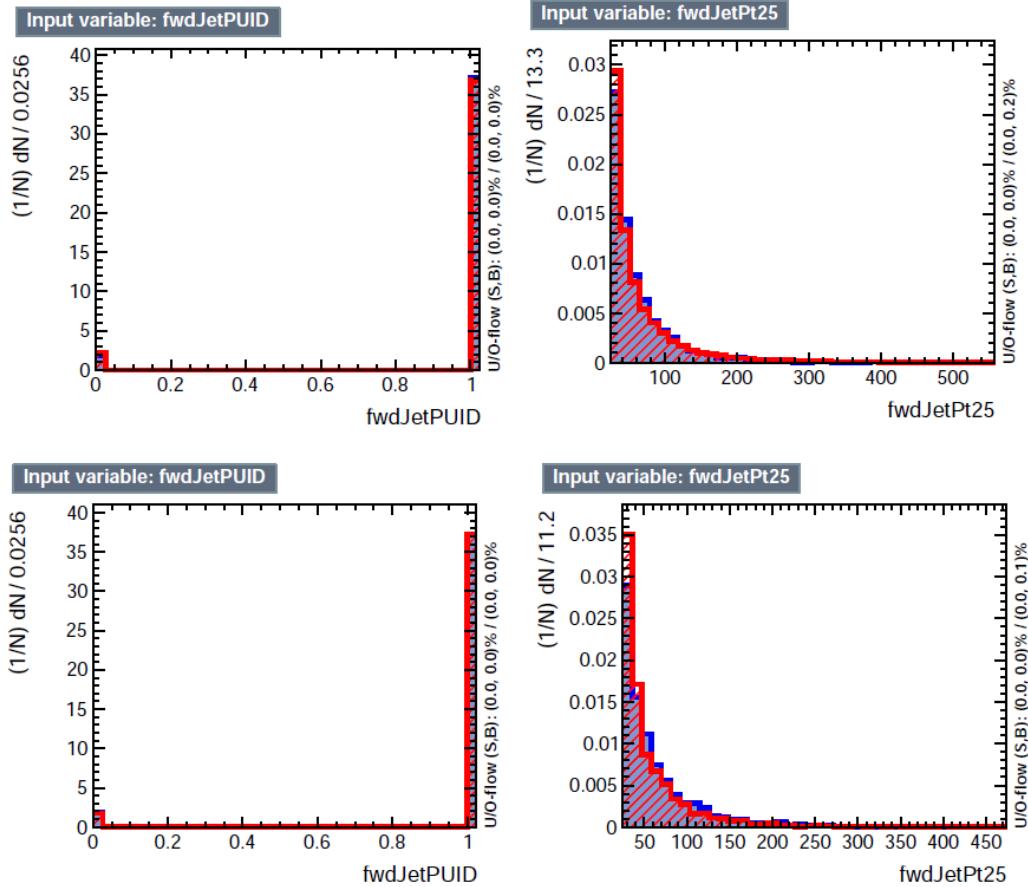


Figure 6.20: Additional discriminating variables distributions for $t\bar{t}V$ training (top row) and $t\bar{t}$ training (bottom row) in the $3l$ channel. The origin of the jets in the forward jet identification distribution is tagged as 0 for *pileup jets* while *primary vertex jets* are tagged as 1.

2970 6.9.5 Signal extraction procedure

2971 Once the two BDTG classifiers, introduced in the previous section, are trained against
 2972 the dominant backgrounds in each channel, they are used to classify the events in the
 2973 samples; their outputs are then used to evaluate the signal cross section limits in a
 2974 fit to the classifier shape. Figure 6.21 shows the expected output distributions in a
 2975 2D plane of one training vs. the other, i.e., $t\bar{t}V$ vs. $t\bar{t}$. Top row shows the 2D planes
 2976 for tHq and tHW signals, while the bottom left plot shows the corresponding 2D

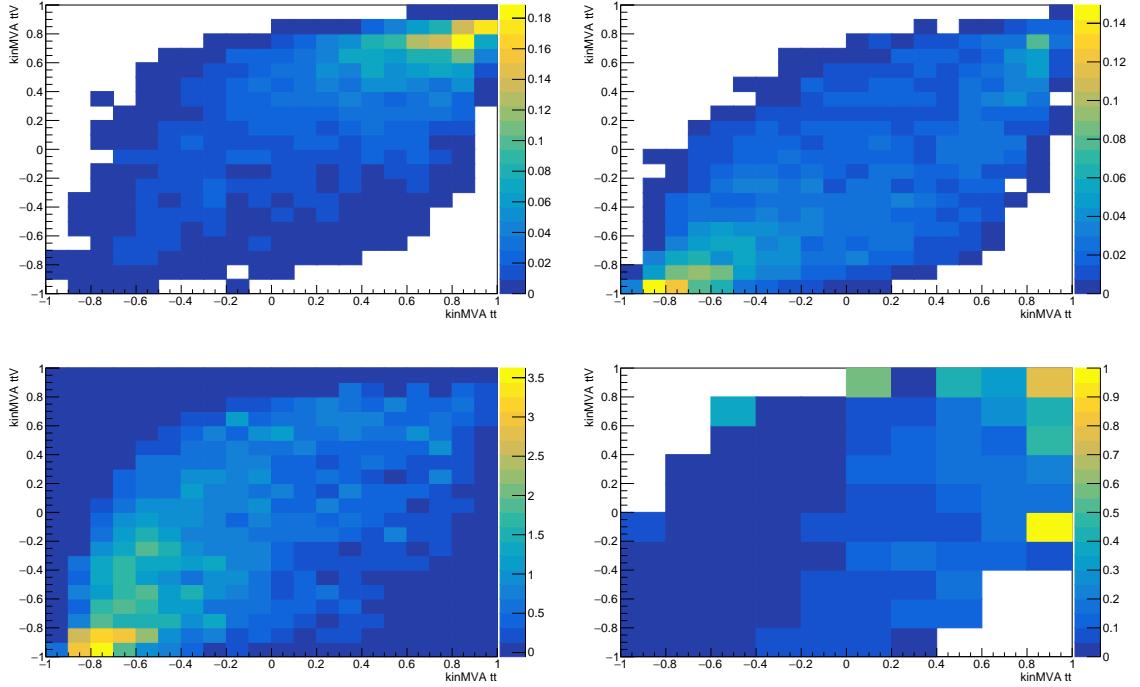


Figure 6.21: BDT classifier output planes (training vs $t\bar{t}$ on x-axis and vs $t\bar{t}V$ on y-axis) for the tHq and tHW signals (top row), and for the combined backgrounds (bottom left). Bottom right: S/B ratio (combining tHq and tHW) in the same plane. Plots are for $3l$ channel.

2977 plane for the combined backgrounds, which are evaluated as in the final background
 2978 prediction, i.e., these are not the samples used in the BDTG training and this includes
 2979 data-driven backgrounds. The signal (combining of tHq and tHW) to background
 2980 ratio (S/B) is showed in the bottom right plot of Figure 6.21.

2981 Each event is now classified into one of ten 2D-bins according to its position in the
 2982 plane, as shown in Figure 6.22. The number of bins is chosen such that no bins are
 2983 entirely empty for any process. The bin boundary positions and number of bins have
 2984 been studied and optimized with respect to the expected limit on the signal strength
 2985 (see Sec. 6.9.6).

2986 From this event categorization, a 1D histogram of expected distribution is pro-
 2987 duced for each signal and background process, and fit to the observed data (or the

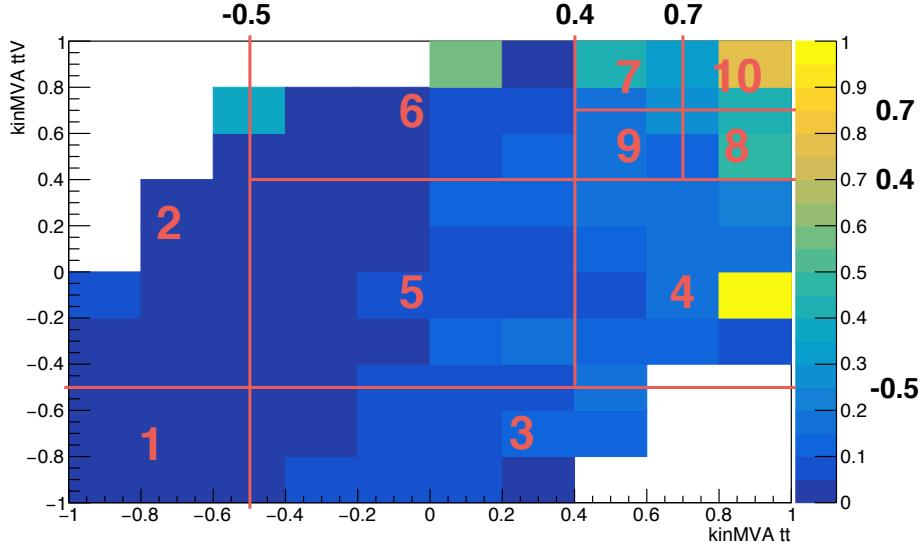


Figure 6.22: Binning overlaid on the S/B ratio map on the plane of classifier outputs.

2988 Asimov dataset for expected limits).

2989 6.9.6 Binning and selection optimization

2990 The effect of the choice of pre-selection cuts and the number of bins of the 1D his-
 2991 togram on the cross section limit is evaluated by varying the most important cuts and
 2992 re-calculating the limit in each case. In this analysis, the optimization was performed
 2993 in the $3l$ channel, by evaluating the upper limits on the $tHq + tHW$ expected signal
 2994 strength only (without $t\bar{t}H$ component), always evaluated at $\kappa_t = -1.0$, $\kappa_V = 1.0$.

2995 Table 6.14 shows the several variations explored, compared with a baseline; the
 2996 baseline is similar to the selection reported in Table 6.6 but only a loose CSV jet and
 2997 a Z veto of ± 10 GeV are required.

2998 The optimal limit is found when requiring a slightly tighter selection with respect
 2999 to the baseline. The optimal selection is reported in Table 6.6.

3000 The signal strength limit also depends on the chosen binning in the 2D plane as
 3001 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 η	$\geq 0 \rightarrow \geq 1$	< 2.94
Light forward jet η	$\geq 0 \rightarrow \geq 1.5$	< 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 ± 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.

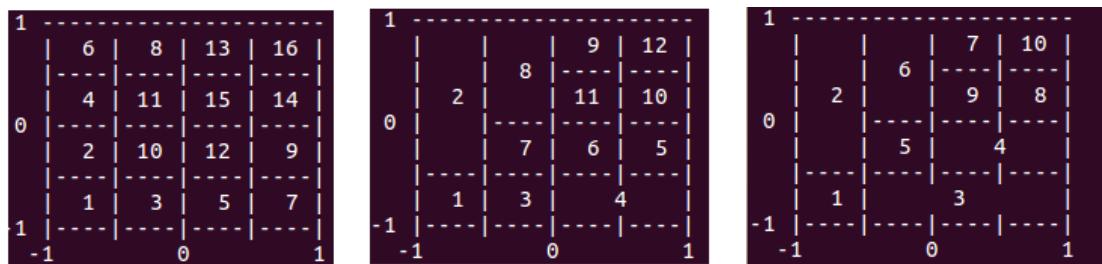


Figure 6.23: Binning combination scheme.

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
10	-0.5	0.4	0.7	-0.5	0.4	0.7	< 2.81

Table 6.15: Limit variation as a function of bin size. The final bin borders used in the $3l$ channel are indicated in bold.

3011 borders and the resulting signal strength limits for the same-sign dimuon channel are
 3012 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
10	-0.3	0.3	0.7	-0.3	0.2	0.6	< 1.69

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.)

3013 The expected limit was found to be **r<1.69** for optimized bin borders in 10 bins
 3014 and optimized pre-selection cuts.

3015 Two additional binning strategies were tested, however, the obtained limits are
 3016 degraded; they are documented in Appendix C.

3017 6.10 Forward jet mismodeling

3018 As said in previous section, among the features of the tHq signature with that serves
 3019 as a powerful discriminating variable is the presence of a forward jet; unfortunately,
 3020 its η distribution is poorly modeled in simulation. To estimate the effect of a mis-
 3021 modeled forward jet distribution, a reweighting of the events in simulation based on
 3022 the normalized data/MC ratio in a control region is performed; as a result, an al-
 3023 ternative shape of the BDT output distributions that reflects a hypothetical perfect
 3024 data/MC agreement is derived.

3025 Using a sample of dileptonic $t\bar{t}$ events, the control region is defined by requiring
 3026 two opposite-sign tight leptons in the $e\mu$ channel, with at least two jets and at least
 3027 one medium CSV tagged jet. (Otherwise the selection is identical to the same-sign
 3028 $e^\pm\mu^\pm$ channel selection). Some distributions related to the forward jet for MC and
 3029 data are shown in Figure 6.24.

3030 The disagreement of the η distribution of forward jets for a p_T cut of 25 GeV is
 3031 well visible especially at higher values of $|\eta|$. The multiplicity for central jets is poorly
 3032 described by the MadgraphMLM sample used here; consistent with other observations
 3033 of the same sample. The $t\bar{t}$ background in this analysis is modeled with a data-driven
 3034 method and these disagreements do not directly affect the $t\bar{t}$ contribution in the
 3035 analysis. They do however reflect the expected agreement in these distributions for
 3036 the irreducible backgrounds and the signal.

3037 The effect of higher p_T cuts on the forward jet has been studied for three values:
 3038 25, 30 and 40 GeV. In order to take into account the data/MC disagreement in the
 3039 high η regions, the events are weighted accordingly to the data/MC ratio of the unity
 3040 normalized control plots shown in Figure 6.25. The data/MC agreement in the
 3041 forward jet η distribution improves significantly at higher jet p_T s.

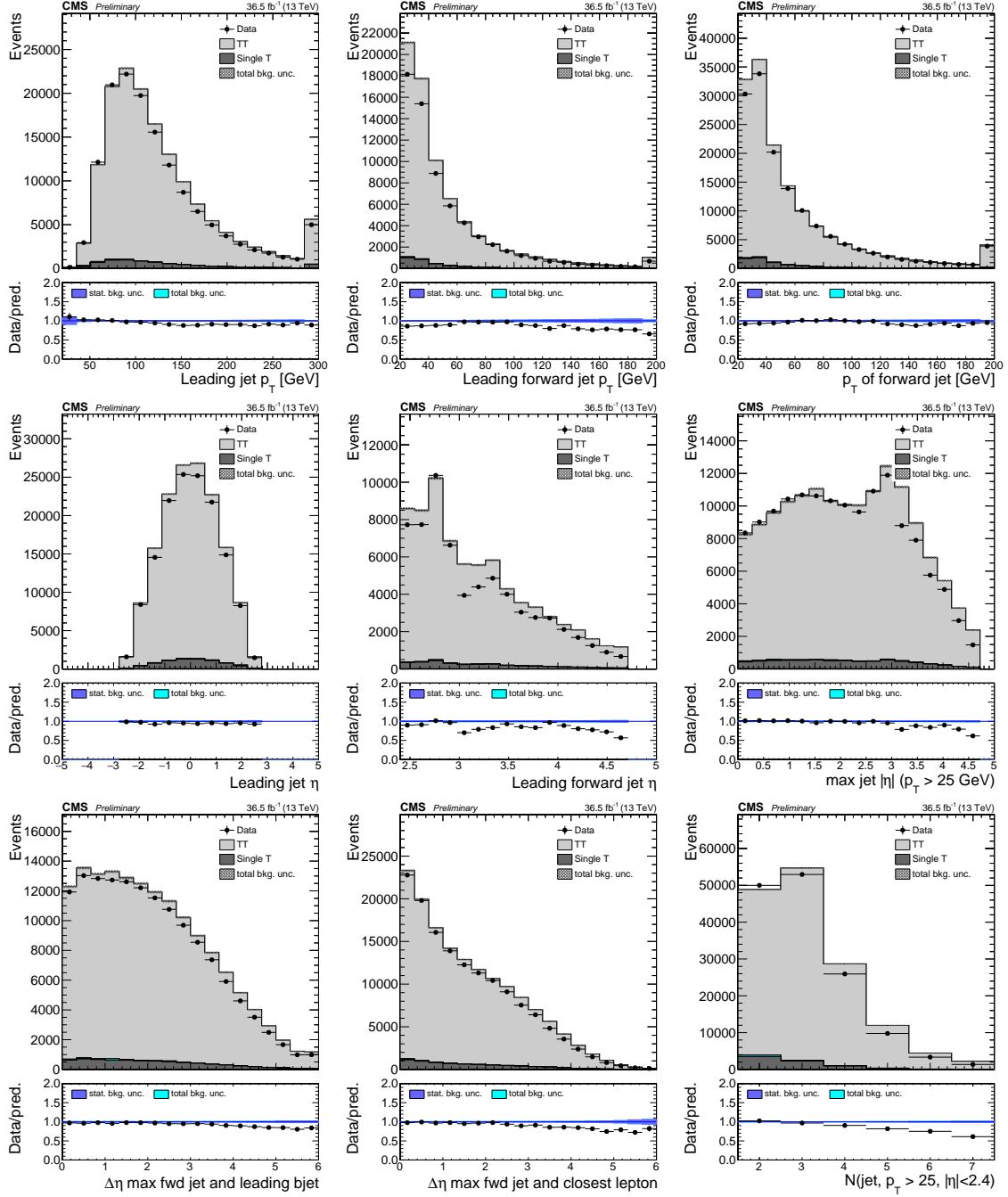


Figure 6.24: Kinematic distributions in the $t\bar{t}$ -enriched opposite-sign $e\mu$ selection. Top row, left to right: leading central ($\eta < 2.4$) jet p_T , leading forward ($\eta > 2.4$) jet p_T , p_T of non-CSV-loose jet with highest η (“light forward jet”). Middle row: η distribution of those 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.

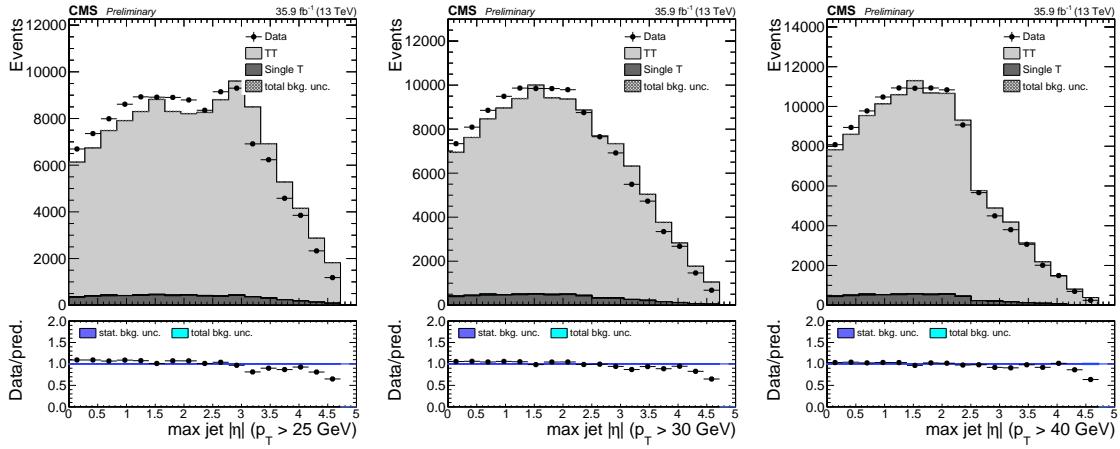


Figure 6.25: Pseudorapidity distributions of the most forward, non-CSV-loose tagged jet in the $t\bar{t}$ -enriched opposite-sign $e\mu$ selection for the three p_T cut values studied.

3042 Table 6.17 shows the scale factors obtained for the three p_T values. The expected
 3043 limit on cross section in the $3l$ was used to determine the most appropriate forward
 3044 jet p_T cut; higher p_T cut improves from 1.54 at 25 GeV to 1.51 at 30 GeV and 1.50
 3045 at 40 GeV. The impact of the data/MC disagreement for forward jet η is observed
 3046 to reduce with higher p_T cuts. Figures F.1, F.2 and F.3 show this reduction in the
 3047 impact of the forward jet η nuisance in the fit.

3048 6.11 Signal model

3049 It is worth to remind that the main goal of this analysis is to test the compatibility
 3050 of points in the parameter space of Higgs-to-vector boson and Higgs-to-top quark
 3051 couplings. This is achieved by using simulated tHq , tHW , and $t\bar{t}H$ signal events
 3052 which are weighted to reflect the impact of the couplings on kinematic distributions,
 3053 and together with different predictions of the respective production cross sections and
 3054 branching ratios, to produce limits on the cross section for different values of κ_V and
 3055 κ_t . See Section 6.4.3 and Table A.3 for the set of κ_t and κ_V values generated. The
 3056 slight shape-dependence of the BDTG classifier outputs as a function of the couplings

η 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 η distribution of most forward, non-tagged jet with three different p_T cuts, see Figure 6.25.

3057 is showed in Appendix D.

3058 In addition to the (κ_t, κ_V) dependence of the tHq and tHW production cross
 3059 sections, due to interferences, the cross section of $t\bar{t}H$ depends quadratically on κ_t
 3060 according to [158]:

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

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

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

3061 The Higgs branching fractions to vector bosons depend on κ_V , and the overall

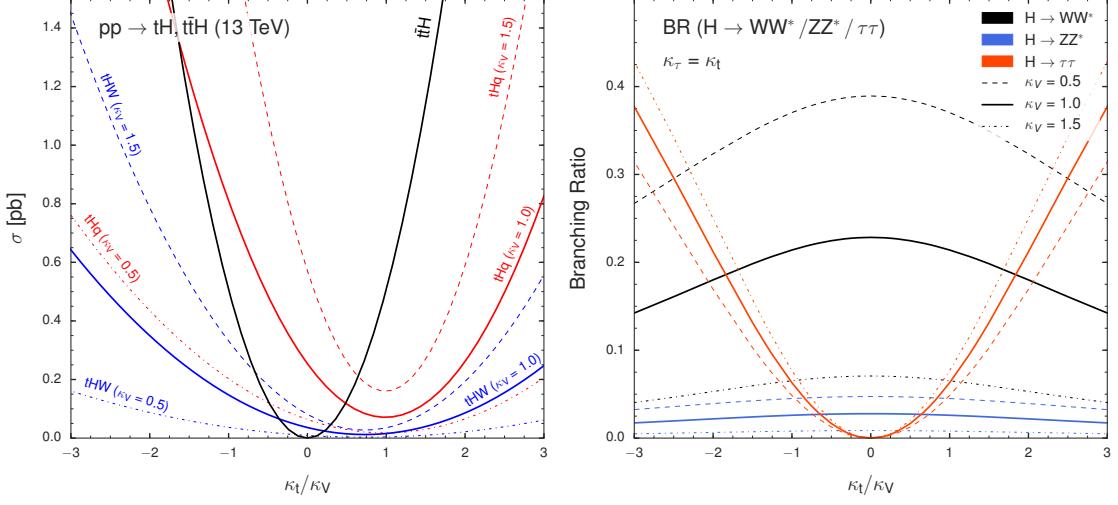


Figure 6.26: Scaling of the tHq , tHW , and $t\bar{H}H$ production cross sections (left) and of the $H \rightarrow WW^*$, $H \rightarrow \tau\tau$, and $H \rightarrow ZZ^*$ branching ratios (right), as a function of κ_t/κ_V , for three different values of κ_V .

3062 Higgs decay width depend both on κ_t and κ_V when considering resolved top-quark
 3063 loops in the $H \rightarrow \gamma\gamma$, $H \rightarrow Z\gamma$, and $H \rightarrow gg$ decays. The relative contributions from
 3064 $H \rightarrow WW$, $H \rightarrow ZZ$, and $H \rightarrow \tau\tau$ also changes with changing κ_V .

3065 If the Higgs-to-tau coupling modifier (κ_τ) is assumed to be equal to κ_t , the relative
 3066 fractions of WW , ZZ , and $\tau\tau$ in the event selection will only depend on the ratio of
 3067 κ_t/κ_V ; thus, any limit set at any given value of κ_t/κ_V is valid for all values of κ_t and
 3068 κ_V with that ratio, and could then be compared with theoretical predictions of cross
 3069 sections at different values of either modifier. Figure 6.26 shows the tHq , tHW and
 3070 $t\bar{H}H$ cross sections(left) and the Higgs boson branching ratios $H \rightarrow WW$, $H \rightarrow ZZ$,
 3071 and $H \rightarrow \tau\tau$ (right) as a function of the κ_t/κ_V ratio.

3072 Thus, this analysis sets an upper limit on the combined cross section times branch-
 3073 ing ratio of tHq , tHW , and $t\bar{H}H$ as a function of the ratio κ_t/κ_V .

3074 Similar interpretation can be made if instead of reporting the limits as a function
 3075 of the κ_t/κ_V ratio, they are reported as a function of the relative strength of Higgs-top
 3076 and Higgs-vector-boson couplings, multiplied by the relative sign

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

3077 this parameter covers the full space between -1.0 and 1.0 , with the SM expectation
 3078 at 0.5 . Absolute values of 1.0 or 0.0 would correspond to purely Higgs-top and purely
 3079 Higgs-V couplings, respectively.

3080 Table 6.18 shows the points in the κ_t/κ_V and f_t parameter space that are mapped
 3081 by the 51 individual κ_t and κ_V points.

3082 The overall Higgs decay width (modified by both κ_t and κ_V) becomes irrelevant
 3083 if limits are quoted as absolute cross sections rather than multiples of the expected
 3084 cross section (which depends on it).

3085 The 1D histograms of events as categorized in regions of the 2D BDTG plane are
 3086 then used in a maximum likelihood fit of signal and background shapes, where the
 3087 tHq , tHW , and $t\bar{t}H$ signals are floating with a common signal strength modifier r ,
 3088 producing a 95% C.L. upper limit the observed cross section of $tHq + tHW + t\bar{t}H$.

3089 This procedure is done separately for each point (κ_t, κ_V) where the cross sections
 3090 and branching fractions are scaled accordingly in each point. Limits at fixed values
 3091 of κ_t/κ_V are by construction identical. Tables G.1–G.3 and G.4–G.6 in Appendix G
 3092 show the scalings of cross section times branching fraction, as well as branching
 3093 fractions alone for each of the Higgs decay modes and each of the signal components.

3094 6.12 Systematic uncertainties

3095 The uncertainties present in this analysis can be either of statistical nature given
 3096 the size of the samples and the probabilistic nature of the processes, or of system-
 3097 atic nature. The systematic uncertainties are associated to theoretical uncertainties
 3098 originating in the limited knowledge of the processes, and also to experimental uncer-

f_t	κ_t/κ_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 κ_t/κ_V and f_t as mapped by the 51 κ_t and κ_V points.

3099 tainties originating for instance from the limited resolution of the detectors. In this
 3100 section, the contributions to the systematic uncertainties from all the sources in this
 3101 analysis are considered.

3102 Rate uncertainties associated to the application of scaling factors for the affected
3103 processes, and shape uncertainties which affect not only the normalization but also
3104 the shape of certain distributions, compose the systematic uncertainties. The latter
3105 can affect the analysis during the event selection; therefore, these systematic shape
3106 uncertainties are applied to the simulation samples.

3107 **Experimental uncertainties.**

3108 • *Luminosity.* The measurement of the luminosity delivered by the LHC is af-
3109 fected by experimental conditions like pileup and the number of protons per
3110 bunch. Due to variations in the LHC running parameters an uncertainty of
3111 2.6% is applied.

3112 • *Lepton efficiencies.* Systematic uncertainties in the signal selection efficiency
3113 arise from correction factors applied to the simulated events in order to better
3114 match the measured detector performance; also from theoretical uncertainties in
3115 the modeling of the signal process. Data/MC differences in the trigger efficiency
3116 accounted with scale factors applied to correct for them, lepton reconstruction
3117 and identification performance, and lepton selection efficiency carry a combined
3118 uncertainty of about 5% per lepton.

3119 • *Jets related uncertainties.* Jet energy corrections affect the uncertainty in the
3120 signal selection efficiency it is evaluated by varying the correction factors within
3121 their uncertainties and propagating the effects to the final results by recalculat-
3122 ing the kinematic quantities. The effects of the jet energy scale uncertainties,
3123 b -tagging efficiency and forward jet mismodeling are evaluated using dedicated
3124 shape templates derived from a variation of the jet energy scale within its uncer-
3125 tainty and from varying the b -tagging forward jet data/MC scale factors within
3126 their uncertainty.

3127 **Theory uncertainties**

3128 The uncertainties from unknown higher orders of tHq and tHW production are
 3129 estimated from a change in the Q^2 scale of double and half the initial value, evaluated
 3130 for each point of κ_t and κ_V . The $t\bar{t}H$ signal component has an uncertainty of about
 3131 $+5.8/\sqrt{s} 9.2\%$ from Q^2 scale variations and a further 3.6% from the knowledge of
 3132 PDFs and α_s [57]. Uncertainties related to the choice of PDF set and its scale are
 3133 estimated to be about 3.7% for tHq and about 4.0% for tHW .

3134 The theoretical uncertainties from unknown higher orders for $t\bar{t}W$ and $t\bar{t}Z$ are 12%
 3135 and 10% respectively; additional uncertainties from the knowledge of PDFs and α_s
 3136 of about 4% each for $t\bar{t}W$ and $t\bar{t}Z$ are estimated.

3137 **Backgrounds**

3138 Besides the theory uncertainties on $t\bar{t}W$ and $t\bar{t}Z$, uncertainties of the smaller irre-
 3139 ducible backgrounds and the charge mis-identification estimate are covered with flat
 3140 normalization uncertainties. The WZ contribution due to the scale factor is derived
 3141 during the background estimation using the control region.

3142 The dominant uncertainty is associated to the estimate of the non-prompt lepton
 3143 contribution using a fake rate method; the main normalization uncertainty comes from
 3144 limited statistics in the data control region, and the subtraction of residual prompt
 3145 lepton contribution as stated in section 6.7.2. Shape variations resembling data/MC
 3146 differences and deviations in closure test are evaluated as shape uncertainties.

3147 **Fake rate closure uncertainties**

3148 In order to determine the systematic uncertainties associated to the fake rates,
 3149 the BDTG classifier output shapes from a pure MC estimation of fake leptons (in
 3150 $t\bar{t}$) and from the application of fake-rates as measured in QCD MC, applied in $t\bar{t}$
 3151 MC events, are compared. The difference in the resulting normalization and output
 3152 shapes, for both trainings vs. $t\bar{t}$ and vs. $t\bar{t}V$, are estimated and propagated to the

3153 fit as normalization and shape variations; Figures 6.27 and 6.28 show the results of
3154 these closure tests.

3155 Table 6.19 list all the systematic uncertainties currently considered in the analysis.

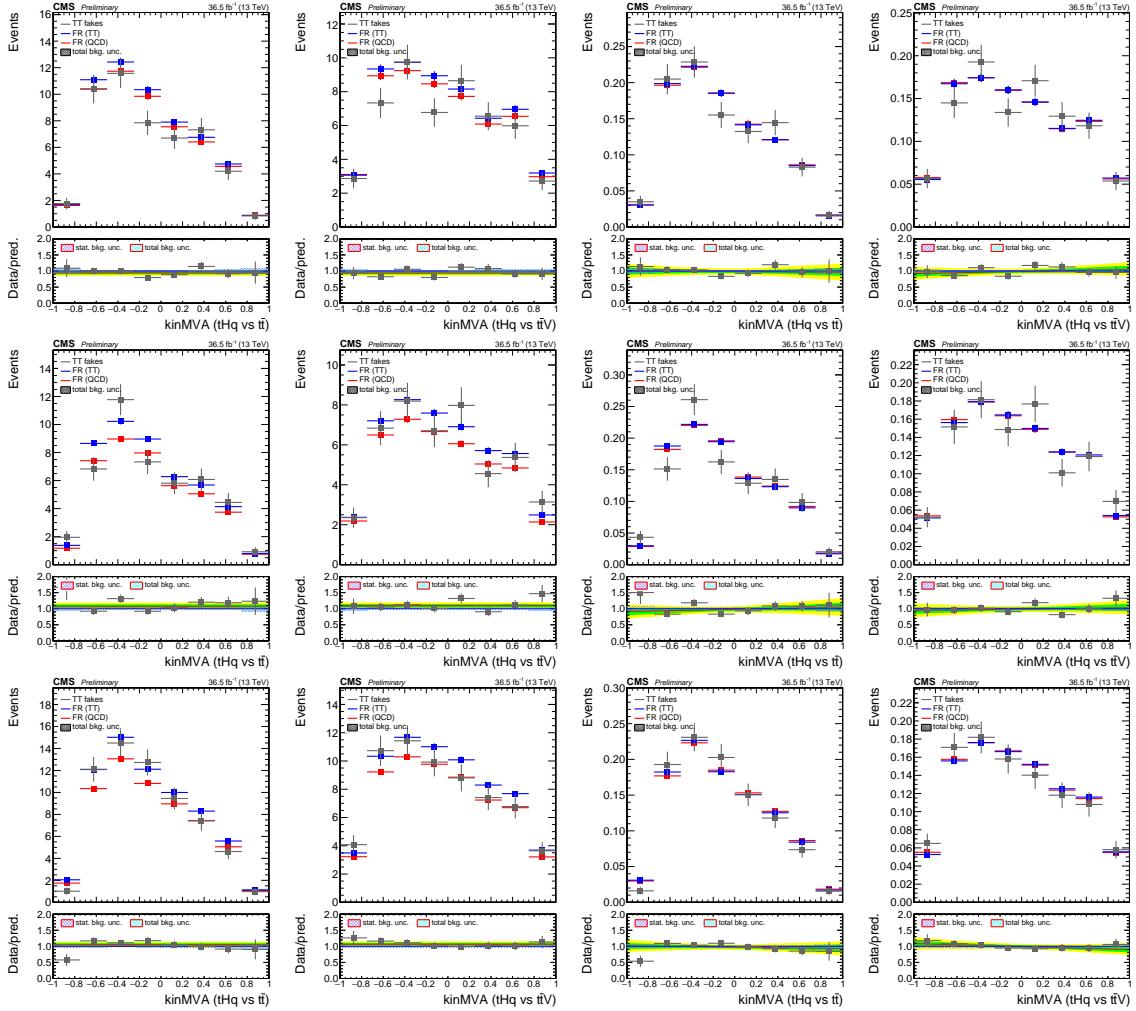


Figure 6.27: BDT outputs comparing $t\bar{t}$ MC to a fake-rate prediction using fake rates measured in QCD MC. Agreement in normalization is estimated from the plots in the two left columns, shape disagreement is estimated from the (normalized) plots in the two right columns. From top to bottom rows: 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.

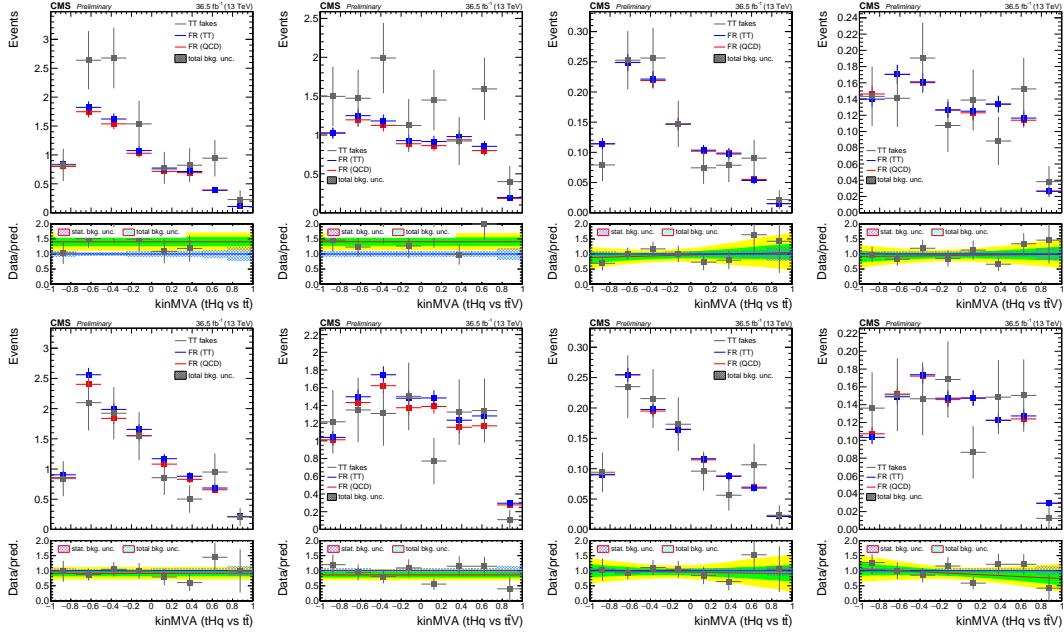


Figure 6.28: BDT outputs comparing $t\bar{t}$ MC to a fake-rate prediction using fake rates measured in QCD MC. Agreement in normalization is estimated from the plots in the two left columns, shape disagreement is estimated from the (normalized) plots in the two right columns. From top to bottom rows: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

Source	Channel	Size
Experimental uncertainties		
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
Theory uncertainties		
Q^2 scale (tHq)	all	0.92–1.06 (depending on κ_t, κ_V)
Q^2 scale (tHW)	all	0.93–1.05 (depending on κ_t, κ_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
Higgs branching fractions		
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
Backgrounds		
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
Fake rate estimate		
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.

3156 6.13 Results

3157 As a result of applying the event pre-selection on the dataset, 127 events are observed
 3158 in the $3l$ channel, 280 in the $2lss \mu^\pm \mu^\pm$ channel and 525 in the $2lss e^\pm \mu^\pm$ channel
 3159 as shown in Table 6.8. These events are then classified into one of ten categories,
 3160 depending on the output of the two BDTG classifiers and according to the optimized
 binning strategy.

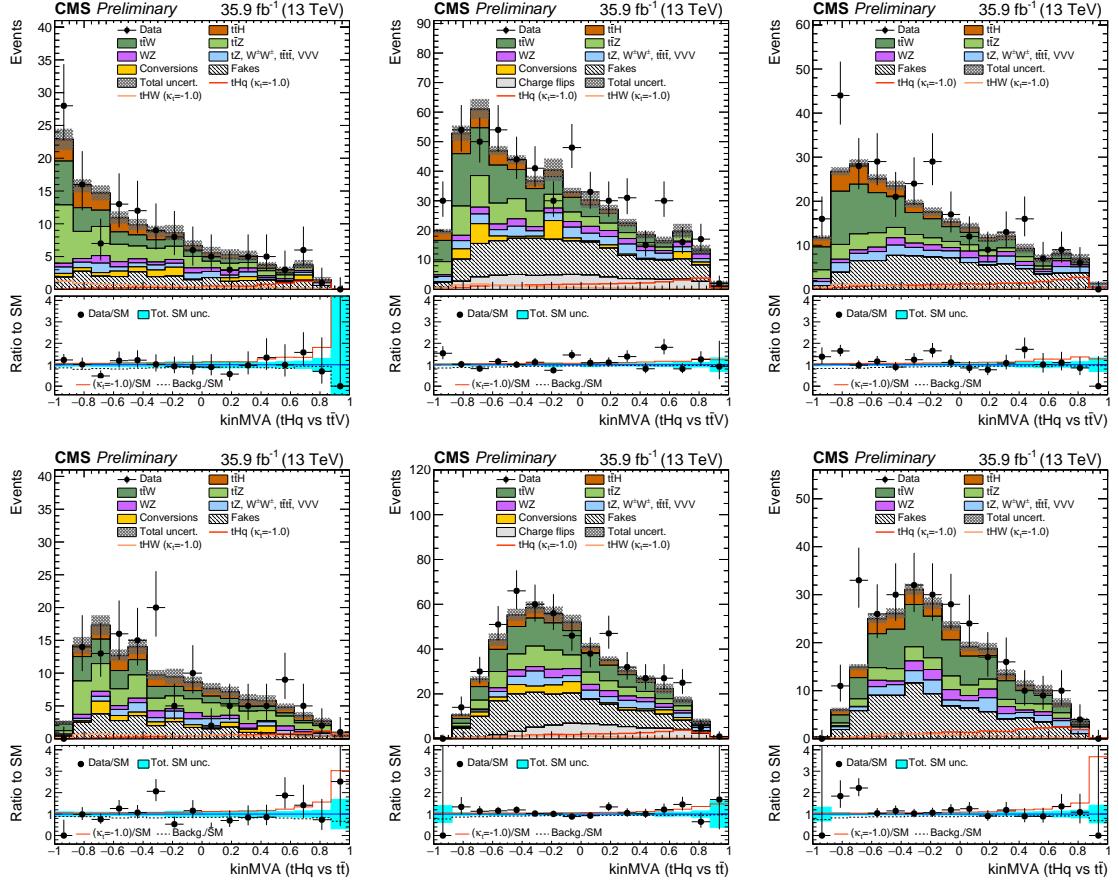


Figure 6.29: Pre-fit BDT classifier outputs, for the three-lepton channel (left), $e^\pm \mu^\pm$ (center), and $\mu^\pm \mu^\pm$ (right), for 35.9 fb^{-1} , for training against $t\bar{t}V$ (top row) and against $t\bar{t}$ (bottom row). In the box below each distribution, the ratio of the observed and 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.

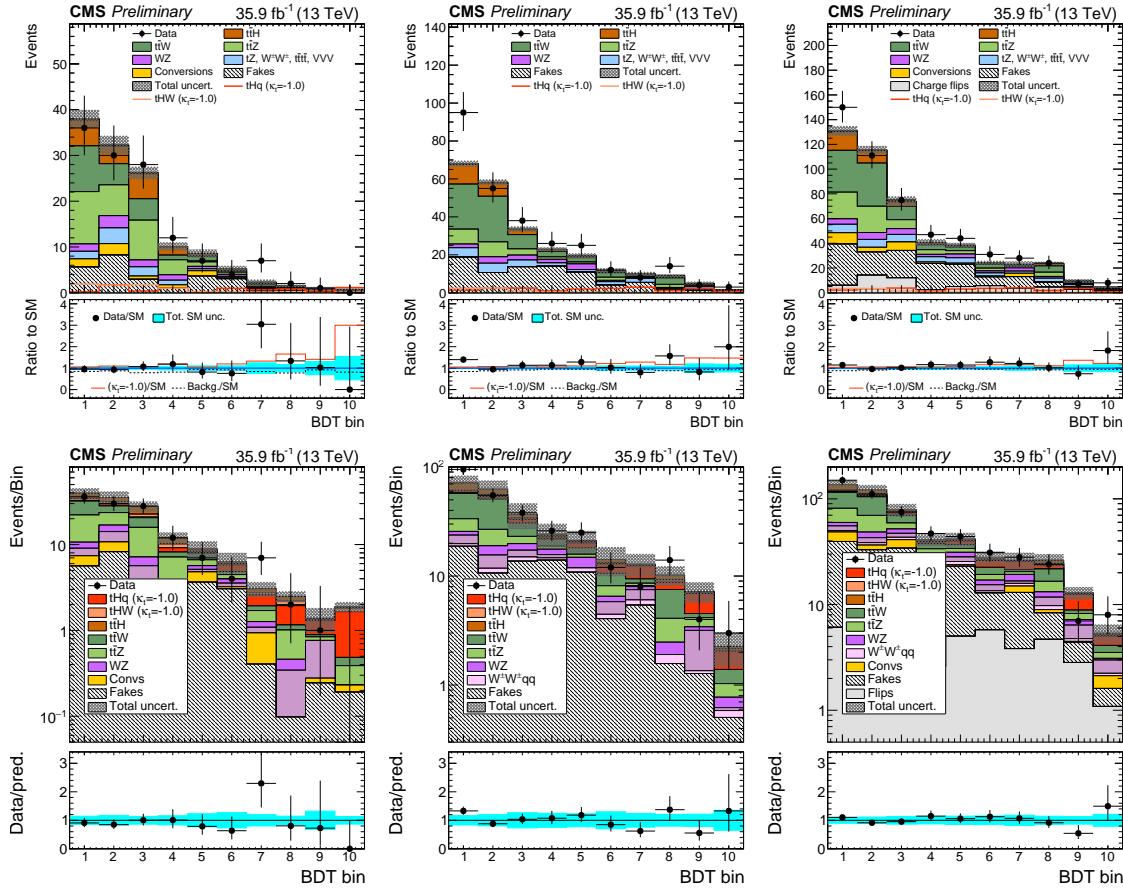


Figure 6.30: Expected (pre-fit) distributions in the final binning used for the signal extraction, for (from left to right) the three lepton channel, the $\mu^{\pm}\mu^{\pm}$ channel, and the $e^{\pm}\mu^{\pm}$ channel. Linear scale (top row), and logarithmic scale (bottom row).

3162 The pre-fit distributions of BDTG outputs are shown in Figure 6.29, while the
 3163 pre-fit distributions in the final binning used in the signal extraction are shown in
 3164 Figure 6.30.

3165 The expected signal and background shapes for the distribution in the one-dimensional
 3166 histogram (with ten bins) are fit to the observed data in a maximum likelihood fit,
 3167 for all three channels simultaneously and separately for the signal shapes for each of
 3168 the 33 κ_t/κ_V coupling configuration points.

3169 The tH and $t\bar{H}$ production cross sections and the Higgs decay branching ratios are
 3170 modified in each point with the Higgs-top (κ_t) and Higgs-vector boson (κ_V) coupling

strength and the Higgs-tau coupling strength modifier (κ_τ) is assumed to be equal to κ_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 κ_t/κ_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.

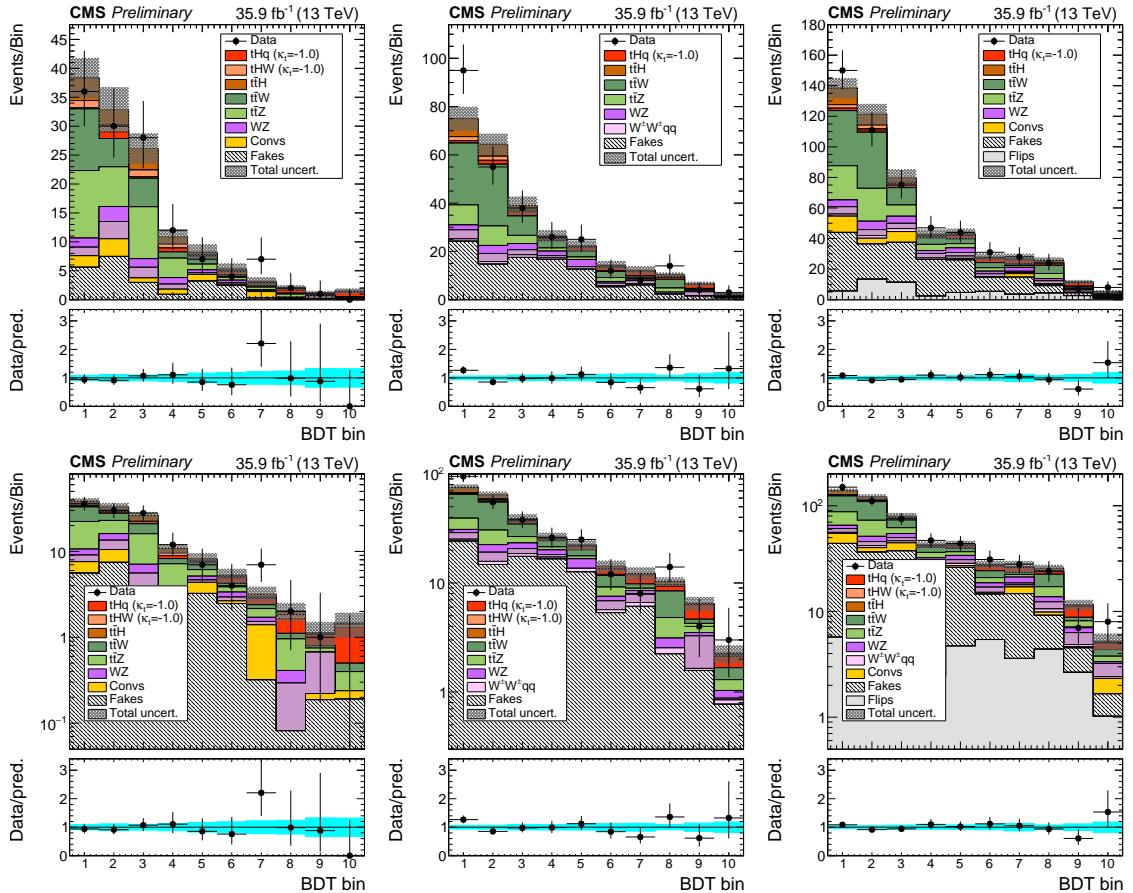


Figure 6.31: Post-fit distributions in the final binning used for the signal extraction, for (from left to right) the three lepton channel, the $\mu^\pm\mu^\pm$ channel, and the $e^\pm\mu^\pm$ channel. Linear scale (top row), and logarithmic scale (bottom row).

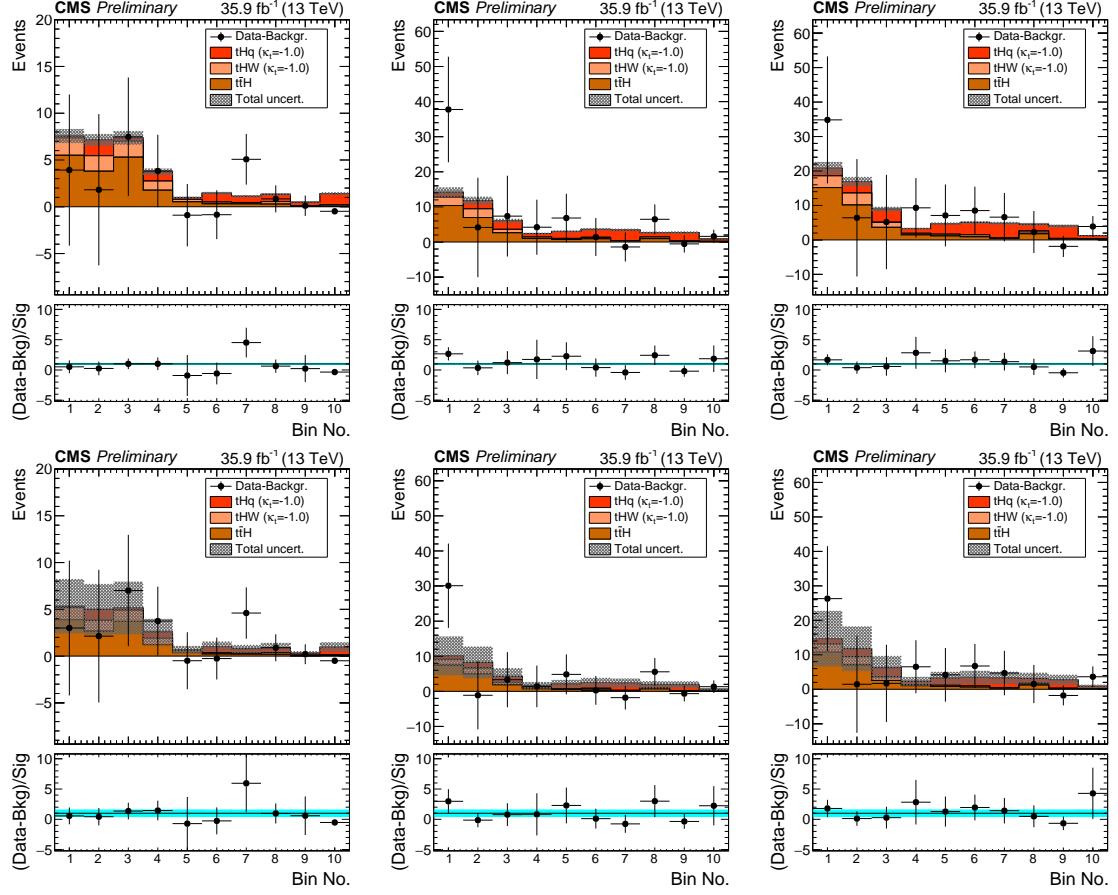


Figure 6.32: Background-subtracted pre- (top) and post-fit (bottom) distributions in the final binning used for the signal extraction, for three lepton channel (left), the $\mu^\pm\mu^\pm$ channel (center), and the $e^\pm\mu^\pm$ channel (right). For a fit in the inverted couplings scenario ($\kappa_V = 1, \kappa_t = -1$).

3180 As expected, the signal contribution is very small compared to the background
 3181 ground contribution; however, it is possible to see the signal contribution by subtracting
 3182 the background from the overall BDT output distributions as shown in Figure
 3183 6.32 for the inverted coupling scenario ($\kappa_V = 1, \kappa_t = -1$) and Figure 6.33 for the SM-like
 3184 scenario ($\kappa_V = 1, \kappa_t = 1$).

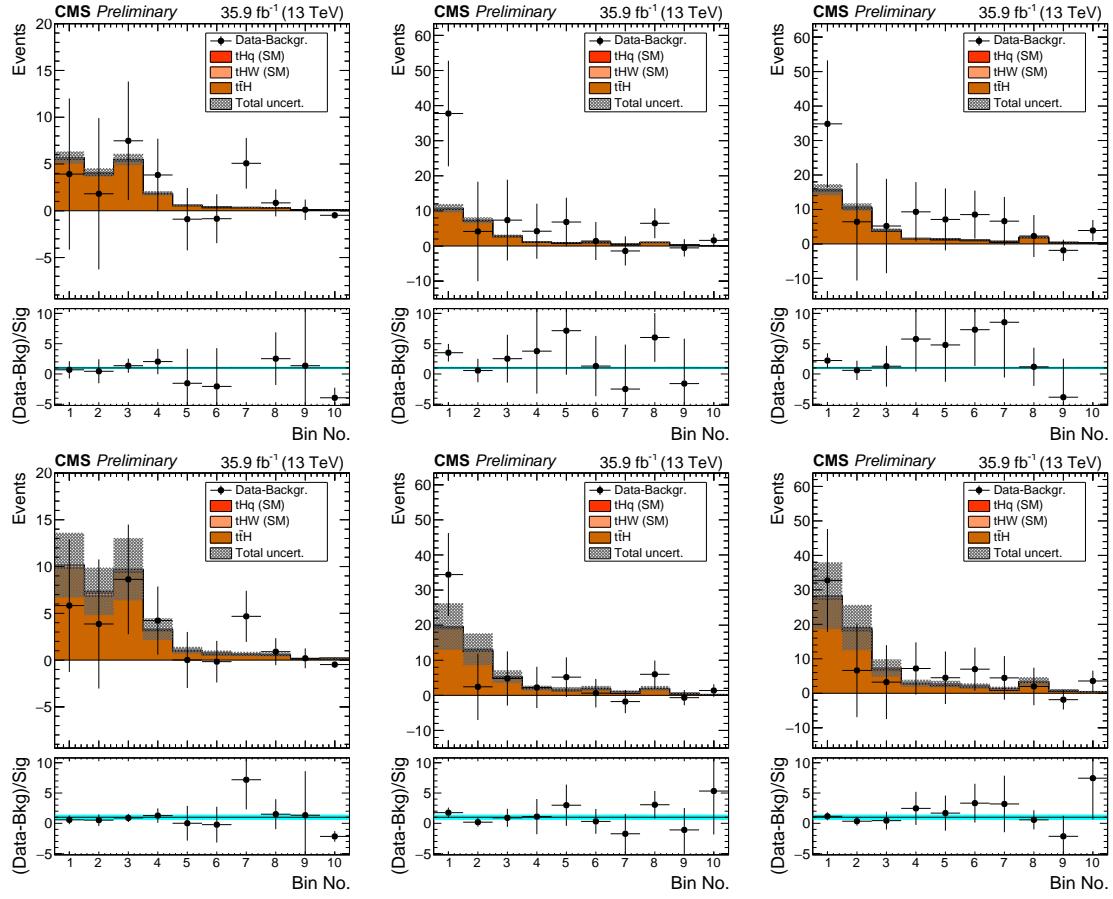


Figure 6.33: Background-subtracted pre- (top) and post-fit (bottom) distributions in the final binning used for the signal extraction, for the three lepton channel (left), the $\mu^\pm\mu^\pm$ channel (center), and the $e^\pm\mu^\pm$ channel (right). For a fit in the SM-like scenario ($\kappa_t = \kappa_V = 1$).

3185 6.13.1 CL_S and cross section limits

3186 Table 6.20 lists the expected background only, the expected SM-like Higgs signal, and
 3187 the observed 95% C.L. upper limits on the $tH + t\bar{t}H$ production cross section times
 3188 $H \rightarrow WW^* + ZZ^* + \tau\tau$ branching ratio (in pb); the corresponding plots are shown
 3189 in Figure 6.34 for $\kappa_V = 1$. The expected background-only limit is calculated on an
 3190 Asimov dataset, while the expected SM-like limit is calculated on an Asimov dataset
 3191 that includes the SM-like tH and $t\bar{t}H$ signals.

3192 An excess of more than 2σ is observed for the SM configuration ($\kappa_t/\kappa_V = 1$) for the

f_t	κ_t/κ_V	Exp. lim.	SM exp.	Obs. lim.	Best fit σ [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 $^{+0.252}_{-0.272}$
-0.500	-1.000	0.315 $^{+0.142}_{-0.093}$	0.450 $^{+0.213}_{-0.160}$	0.638	0.304 $^{+0.175}_{-0.176}$	0.685 $^{+0.395}_{-0.396}$
-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 $^{+0.999}_{-1.022}$
0.500	1.000	0.244 $^{+0.105}_{-0.072}$	0.401 $^{+0.154}_{-0.137}$	0.562	0.328 $^{+0.118}_{-0.121}$	1.821 $^{+0.657}_{-0.671}$
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 κ_t/κ_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 1σ ; 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

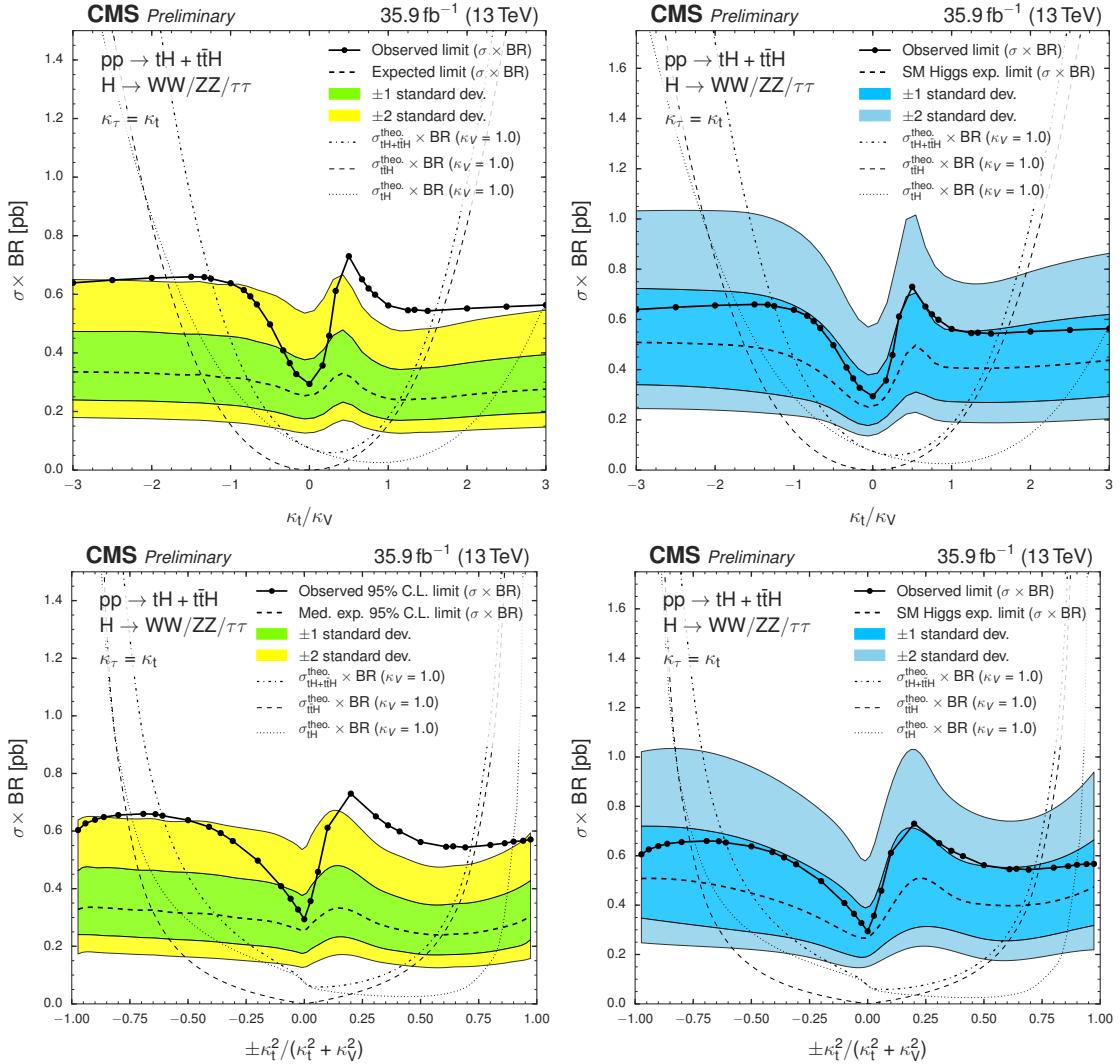


Figure 6.34: Left (Right): Expected background-only (SM-like including $t\bar{t}H$ and tH signals) and observed asymptotic limits on the combined $tH + t\bar{t}H$ cross section times modified BR as a function of κ_t/κ_V (top) and $\text{sign}(\kappa_t/\kappa_V) \times \frac{\kappa_t^2}{(\kappa_t^2 + \kappa_V^2)}$ (bottom) for the combination of three lepton channel, $\mu^\pm\mu^\pm$, and $e^\pm\mu^\pm$ channel.

3197 deviation of the observed limit from the expected one is much smaller than 1σ ; this is
 3198 consistent with the results presented in Reference [149]. It is also evident that, given
 3199 the dependence of the $t\bar{t}H$ cross section on κ_t^2 , the source of the asymmetry in both,
 3200 background-only and SM-like, limits is induced by the tH component of the signal.

3201 Comparing the observed upper limit with the theoretical prediction of the $tH +$

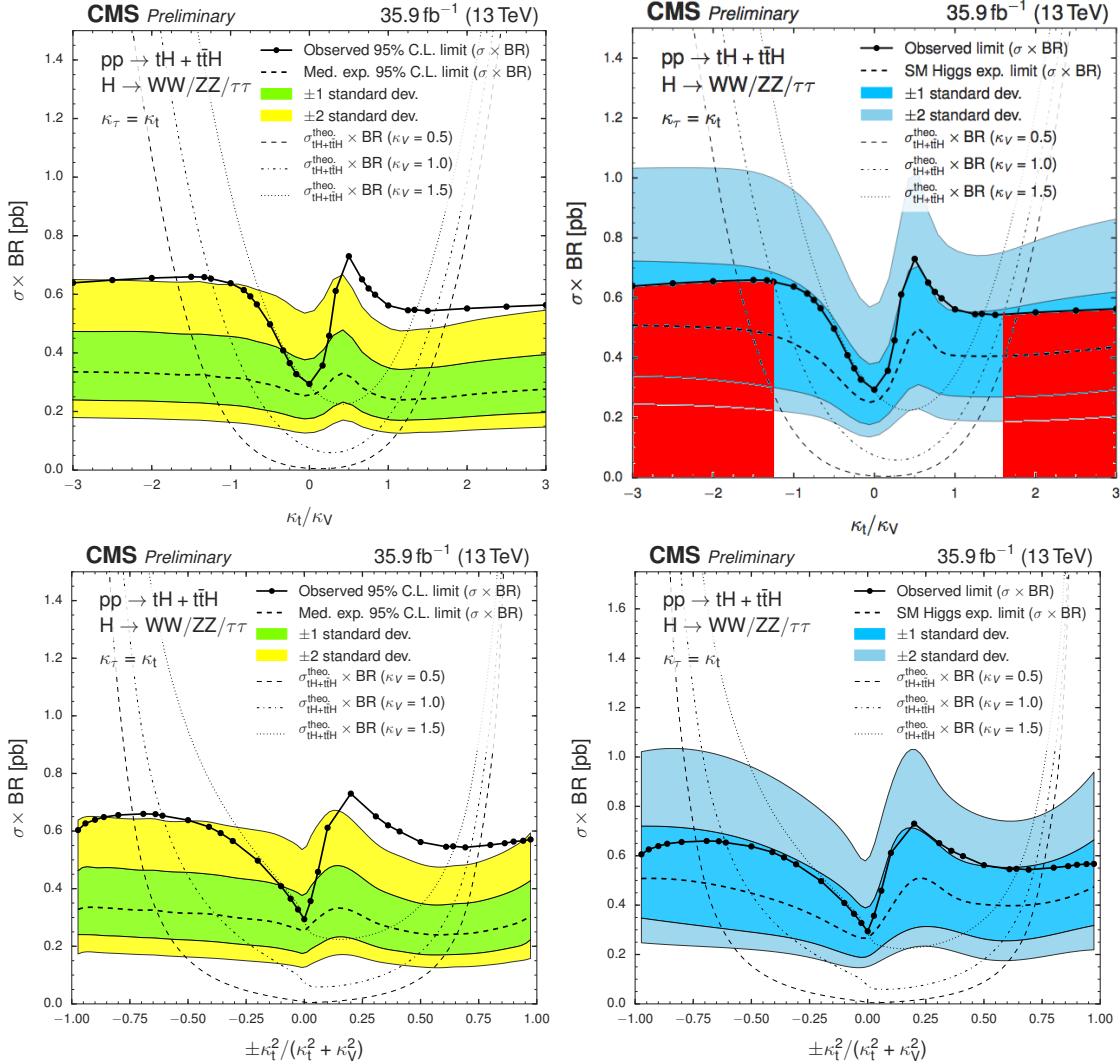


Figure 6.35: Left (Right): Expected background-only (SM-like including $t\bar{t}H$ and tH signals) and observed asymptotic limits on the combined $tH + t\bar{t}H$ cross section times modified BR as a function of κ_t/κ_V (top) and $\text{sign}(\kappa_t/\kappa_V) \times \frac{\kappa_t^2}{(\kappa_t^2 + \kappa_V^2)}$ (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.

3202 $t\bar{t}H$ cross section times BR for $\kappa_V = 1.0$ constrains the allowed range of coupling
 3203 configurations κ_t/κ_V to between about -1.25 and +1.60. as shown in the top right
 3204 plot in Figure 6.35.

3205 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	0.64	0.32	[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	0.56	0.24	[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				
			-2σ	-1σ	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 ($\mu\mu, 3\ell$)	1.6	0.40	0.54	0.78	1.12	1.57
	Combined ($\mu\mu, e\mu, 3\ell$)	1.4	0.37	0.50	0.71	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 ($\mu\mu, 3\ell$)	3.4	0.79	1.07	1.51	2.17	3.01
	Combined ($\mu\mu, e\mu, 3\ell$)	3.1	0.71	0.96	1.36	1.94	2.70

Table 6.22: Expected and observed CL_S 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

3211 Table 6.21, whereas, the summary of the expected and observed CL_S limits (at 95%
 3212 C.L.) on the signal strength of combined $tH + t\bar{t}H$ production in each channel, and
 3213 for different combinations thereof, for the ITC and SM-like scenarios are presented in
 3214 Table 6.22.

3215 **6.13.2 Best fit**

3216 The best-fit results for the signal strength in all the 33 κ_t/κ_V configurations are also
 3217 listed in Table 6.20; the inverted top coupling (ITC) and the SM-like scenarios are
 3218 highlighted there and summarized in Table 6.23. The individual contributions from
 3219 all the channels to the best-fit signal strength for the SM-like Higgs signal are listed
 3220 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 ± 0.40	0.30 ± 0.18 pb	$1.70\sigma(2.51\sigma)$
$\kappa_t/\kappa_V = 1.0$	$1.82^{+0.66}_{-0.67}$	0.33 ± 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.

3221 In the SM scenario, a signal strength of 1.82 is obtained which corresponds to
 3222 a cross section of 0.33pb. The observed significance of the signal, in a background-
 3223 only hypothesis, is 2.7σ , with an a-priori expected significance of 1.5σ . For the
 3224 ITC scenario, the best fit signal strength is 0.68 , corresponding to a significance

of 1.7σ (2.5σ expected); a scan of the observed and expected significances over the κ_t/κ_V configurations is shown in Fig. 6.36. Note that the fit favors a signal strength compatible with zero for a scenario with $\kappa_t = 0$ (where the $t\bar{t}H$ component vanishes).

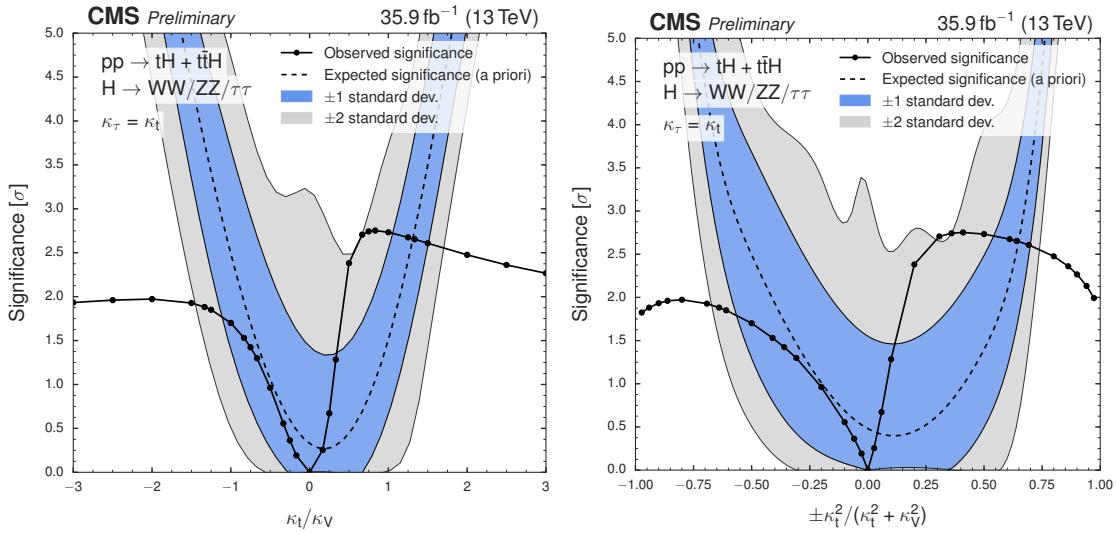


Figure 6.36: Observed and a priori expected significance of the fit result (in a background-only hypothesis) as a function of κ_t/κ_V (top) and f_t (bottom) for the combination of three lepton channel, $\mu^\pm\mu^\pm$, and $e^\pm\mu^\pm$ channel.

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

6.13.3 Effect of the nuisance parameters

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

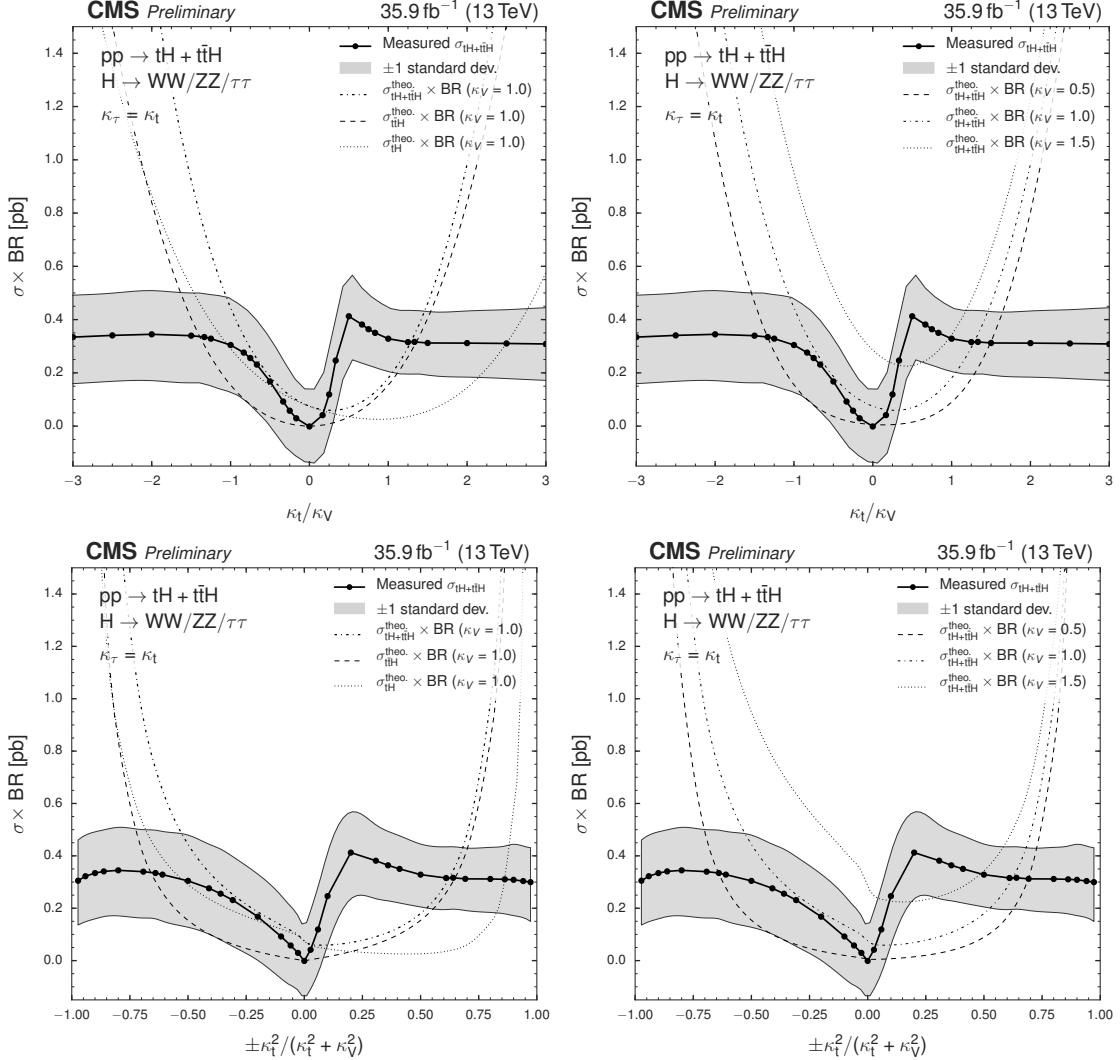


Figure 6.37: Best fit values of the combined $tH + t\bar{H}$ cross section times modified BR as a function of κ_t/κ_V (top) and $\text{sign}(\kappa_t/\kappa_V) \times \frac{\kappa_t^2}{(\kappa_t^2 + \kappa_V^2)}$ (bottom) for the combination of three lepton channel, $\mu^\pm\mu^\pm$, and $e^\pm\mu^\pm$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

3237 Most of the nuisance parameters stay close to their initial values. The biggest
 3238 impact on the signal strength limits is associated to the fake rates for muons, followed
 3239 by the lepton efficiencies and nuisances associated to the QCD scales. The lower
 3240 impact in the ITC scenario is associated to the b-tag and tHq closure normalization
 3241 and shape nuisances, while in the SM scenario, nuisances associated to the forward
 3242 jet in tHq and p.d.f.s have the lower impact in the signal strength limit .

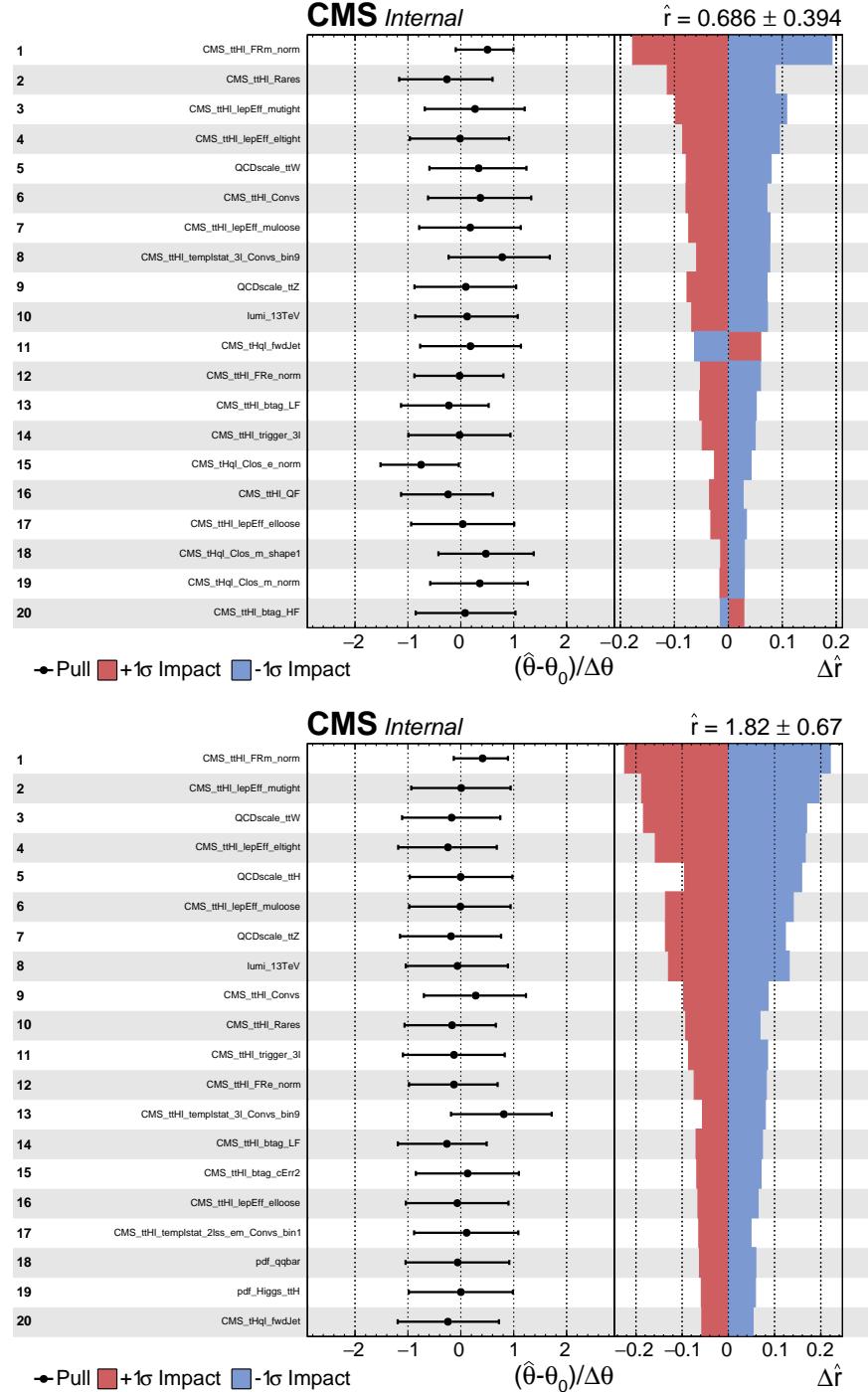


Figure 6.38: Post-fit pulls and impacts of the 20 nuisance parameters with largest impacts for the fit on the observed data, for the ITC (top) and SM (bottom) hypotheses.

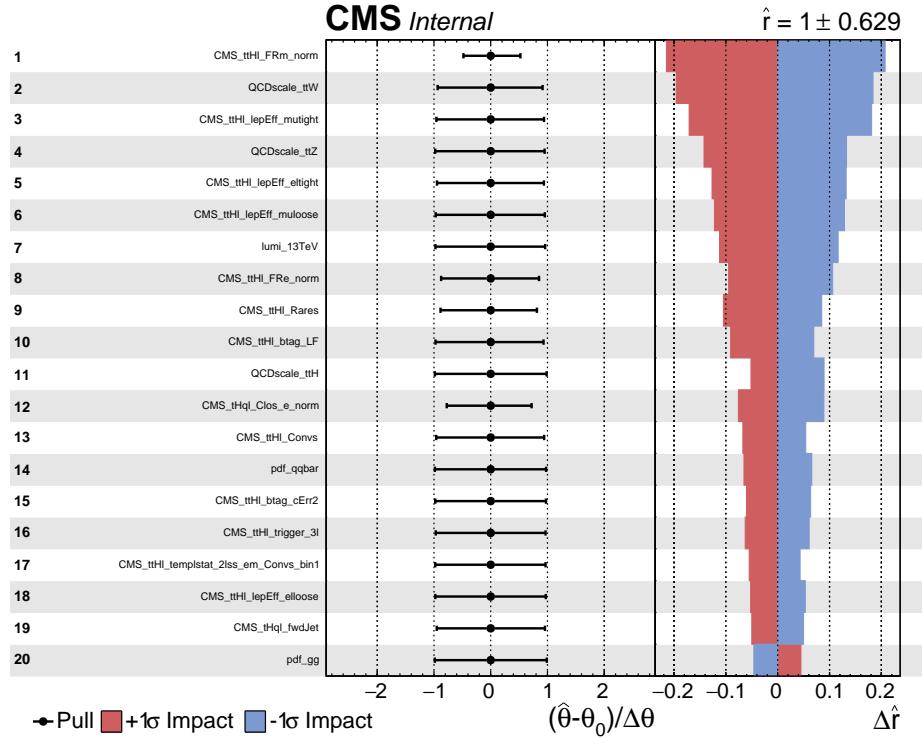


Figure 6.39: Post-fit pulls and impacts of the 20 nuisance parameters with largest impacts for a fit to the Asimov dataset with fixed signal strength, for the $\kappa_t/\kappa_V = -1.0$ hypothesis.

3243 The sensitivity of the analysis is limited by systematic uncertainties, predomi-
 3244 nantly by those concerning the normalizations of the main background components,
 3245 i.e., the non-prompt lepton estimation, the scale uncertainties for $t\bar{W}$ and $t\bar{Z}$, as well
 3246 as by the uncertainties on the measured lepton efficiency.

3247 **6.14 CP-mixing in tHq**

3248 The sensitivity of the tH production process to the CP-mixing in the Higgs boson
 3249 sector was explored in Section 1.6; the theoretical model postulates the existence of a
 3250 generic spin-0 particle X_0 with CP-symmetry violating interaction with the top quark
 3251 but SM-like interaction with the W boson.

3252 The LHE reweighting procedure used in the ITC analysis is used in this CP-mixing

analysis; thus, a tX_0q simulation sample was produced, containing 21 event weights for different CP-mixing angles (α) ranging from values of $\cos\alpha = 1$ to $\cos\alpha = -1$ 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 cross section is scaled to its NLO prediction.

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.

³²⁶¹ **Appendix A**

³²⁶² **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>		
κ_V	κ_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: κ_V and κ_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	σ [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_tW1l_5f_L0_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.

³²⁶³ **Appendix B**

³²⁶⁴ **Aditional plots**

³²⁶⁵ **B.1 Pre-selection kinematic variables**

³²⁶⁶ Figures B.1, B.2 and B.3 show the distributions of some relevant kinematic variables,
³²⁶⁷ normalized to the cross section of the respective processes and to the integrated
³²⁶⁸ luminosity.

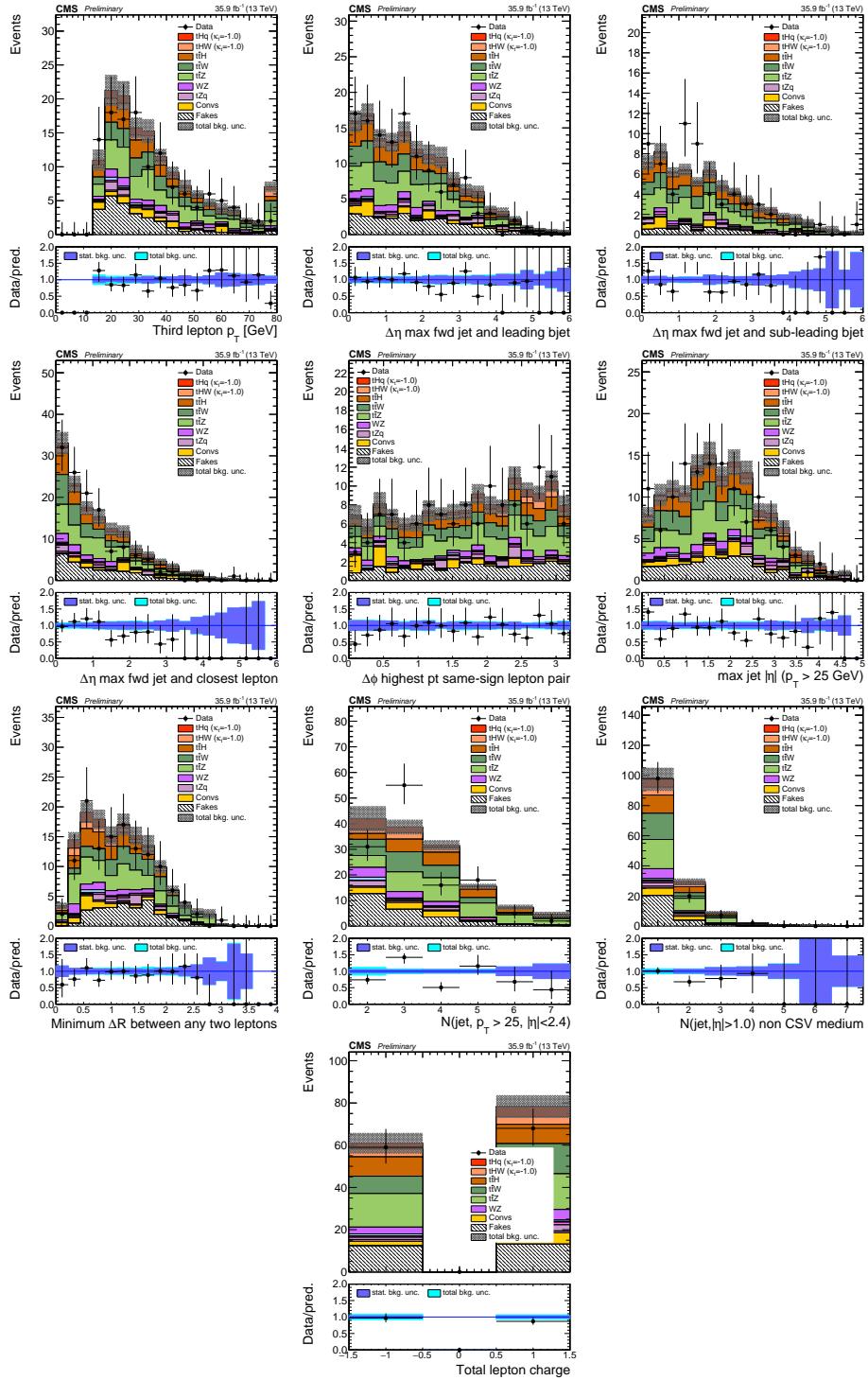


Figure B.1: Distributions of input variables to the BDT for signal discrimination, three lepton channel, normalized to their cross section and to 35.9 fb^{-1} .

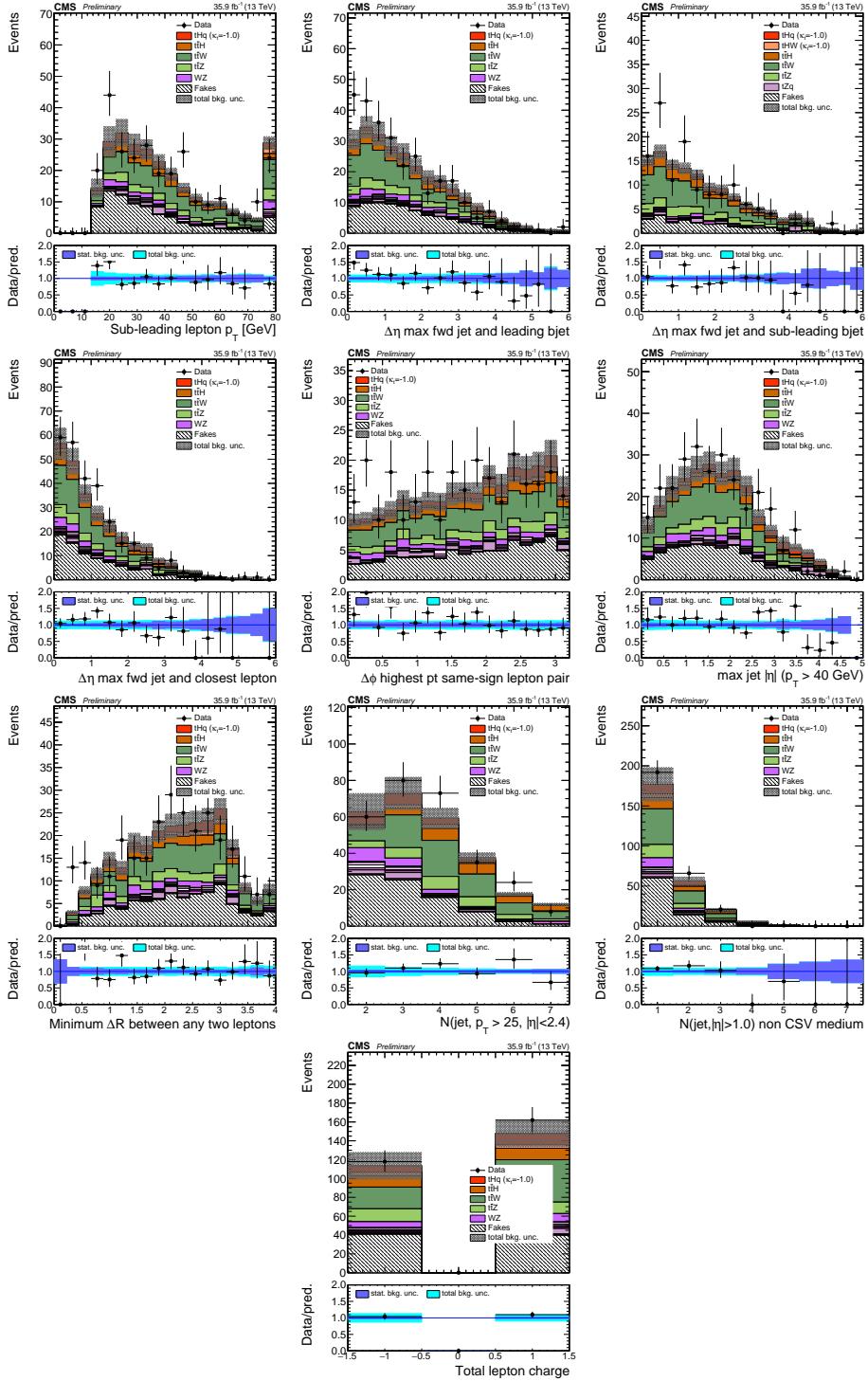


Figure B.2: Distributions of input variables to the BDT for signal discrimination, in $\mu^\pm\mu^\pm$ channel, normalized to their cross section and to 35.9fb^{-1} .

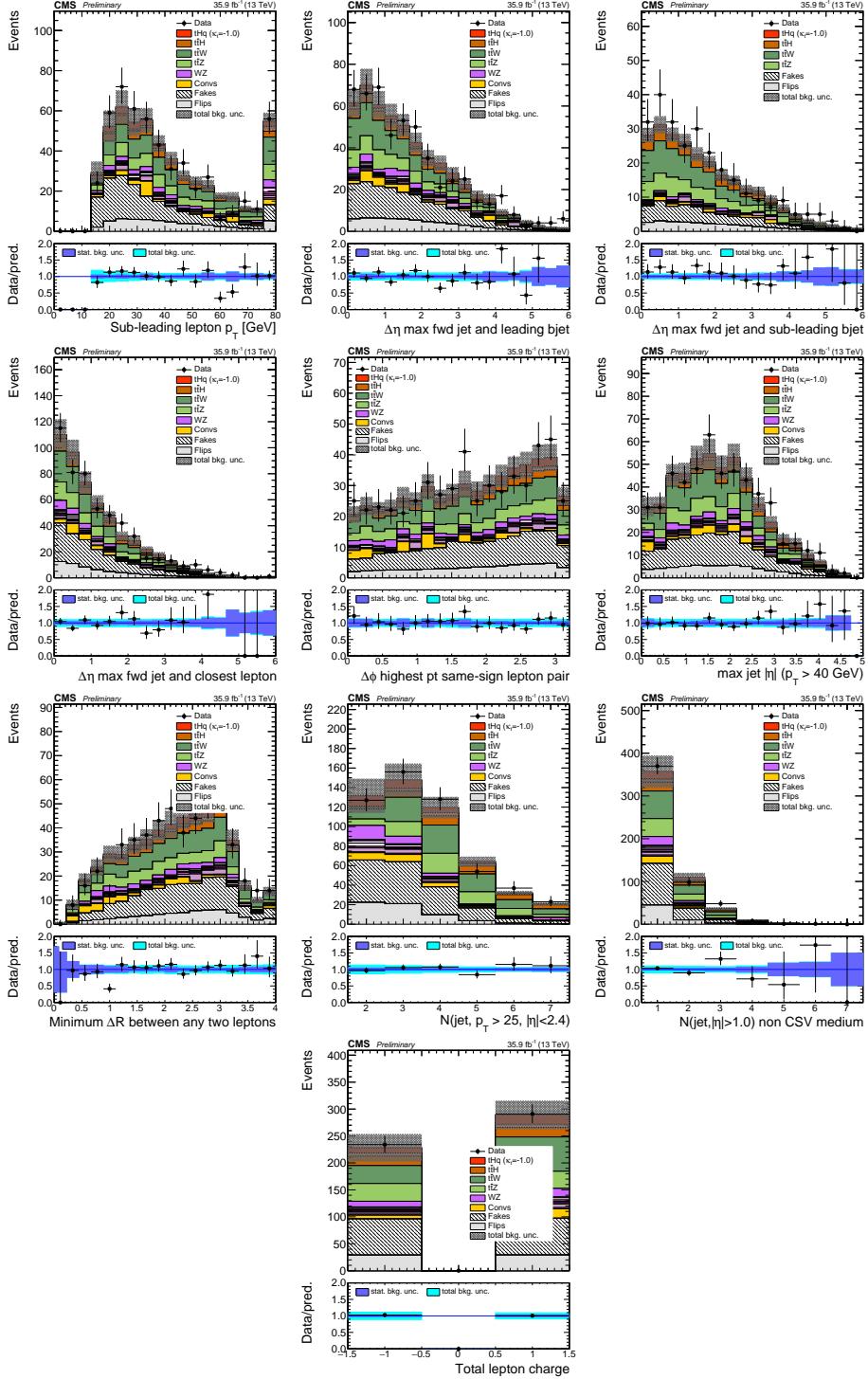


Figure B.3: Distributions of input variables to the BDT for signal discrimination, in $e^\pm\mu^\pm$ channel, normalized to their cross section and to 35.9 fb^{-1} .

3269 **B.2 BDTG input variables for $2lss$ channel**

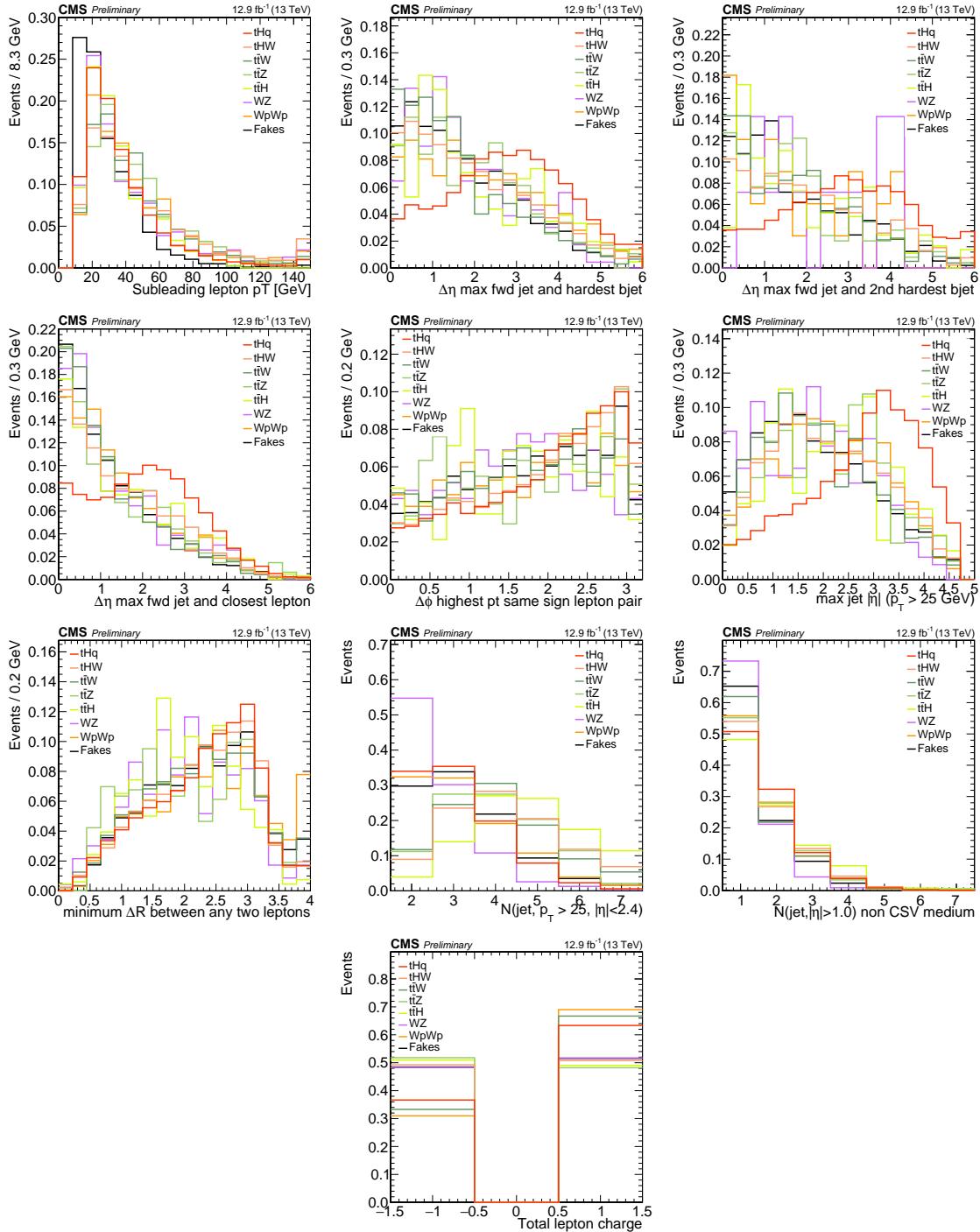


Figure B.4: Distributions of input variables to the BDT for signal discrimination, two lepton same sign channel.

3270 **B.3 Input variables distributions from BDTG**
 3271 classifiers

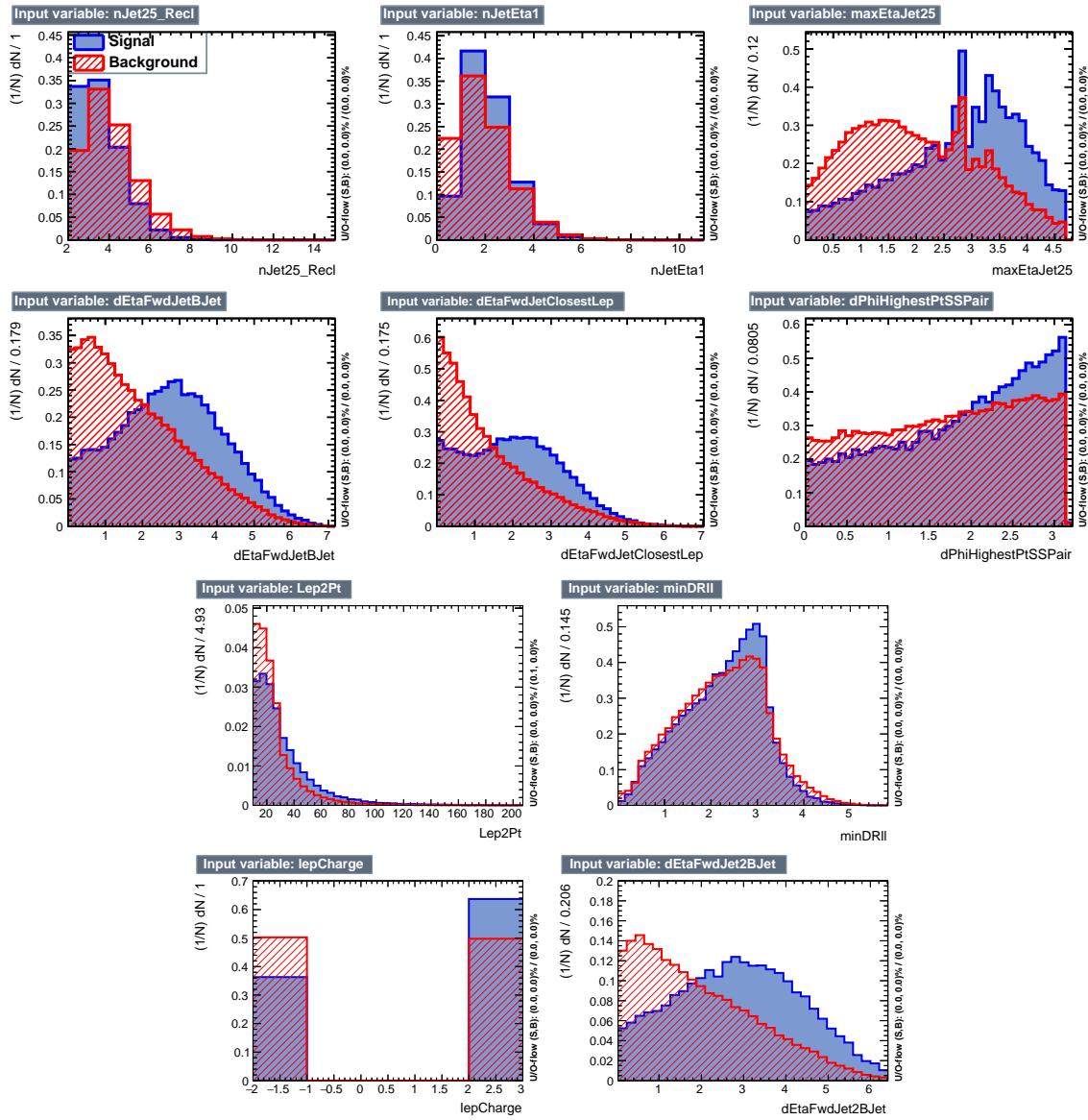


Figure B.5: BDT input variables as seen by BDTG classifier for the $2lss$ channel, tHq signal (blue) discriminated against $t\bar{t}$ background (red).

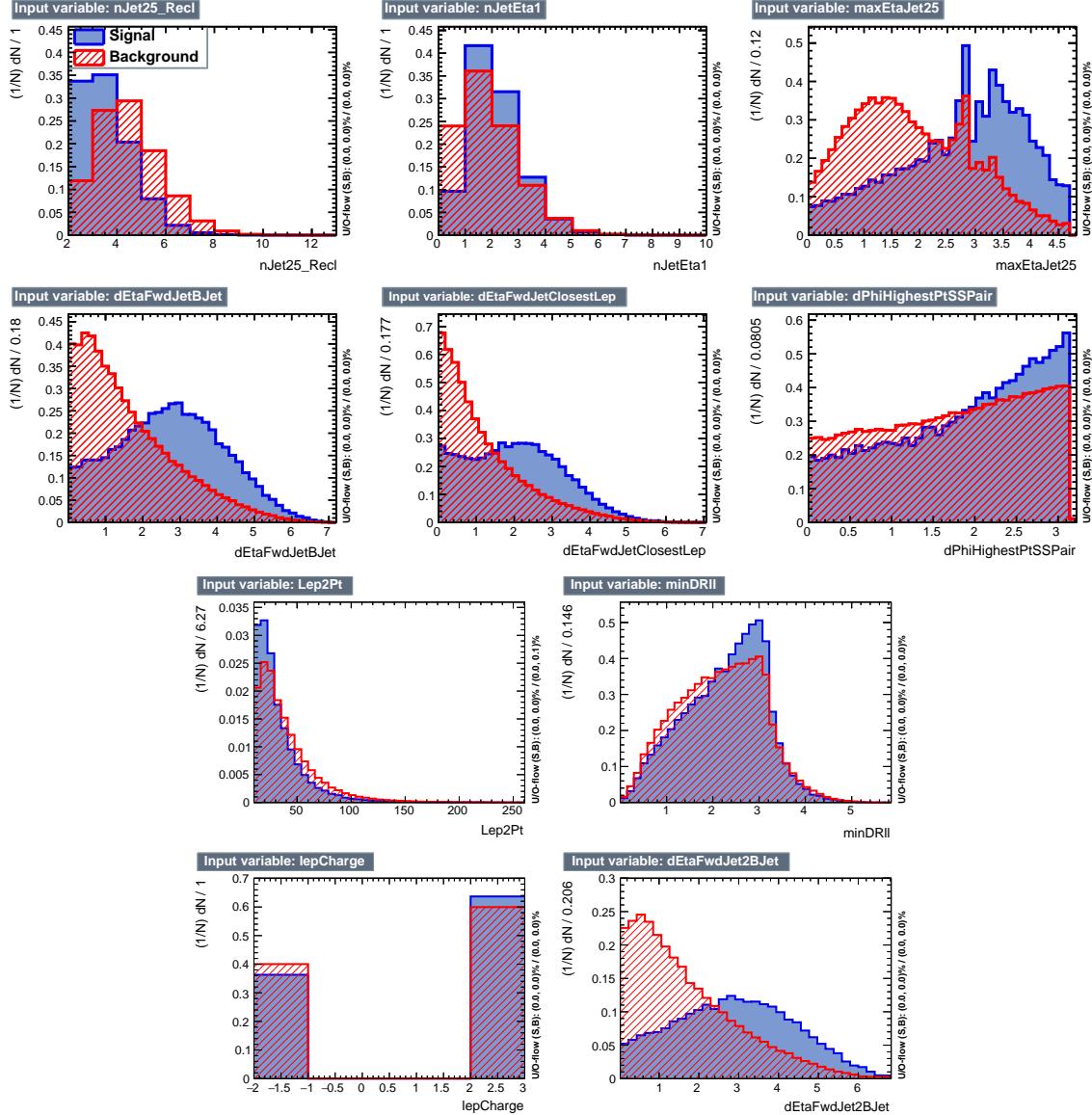


Figure B.6: BDT input variables as seen by BDTG classifier for the $2lss$ channel, tHq signal(blue) discriminated against $t\bar{t}V$ background (red).

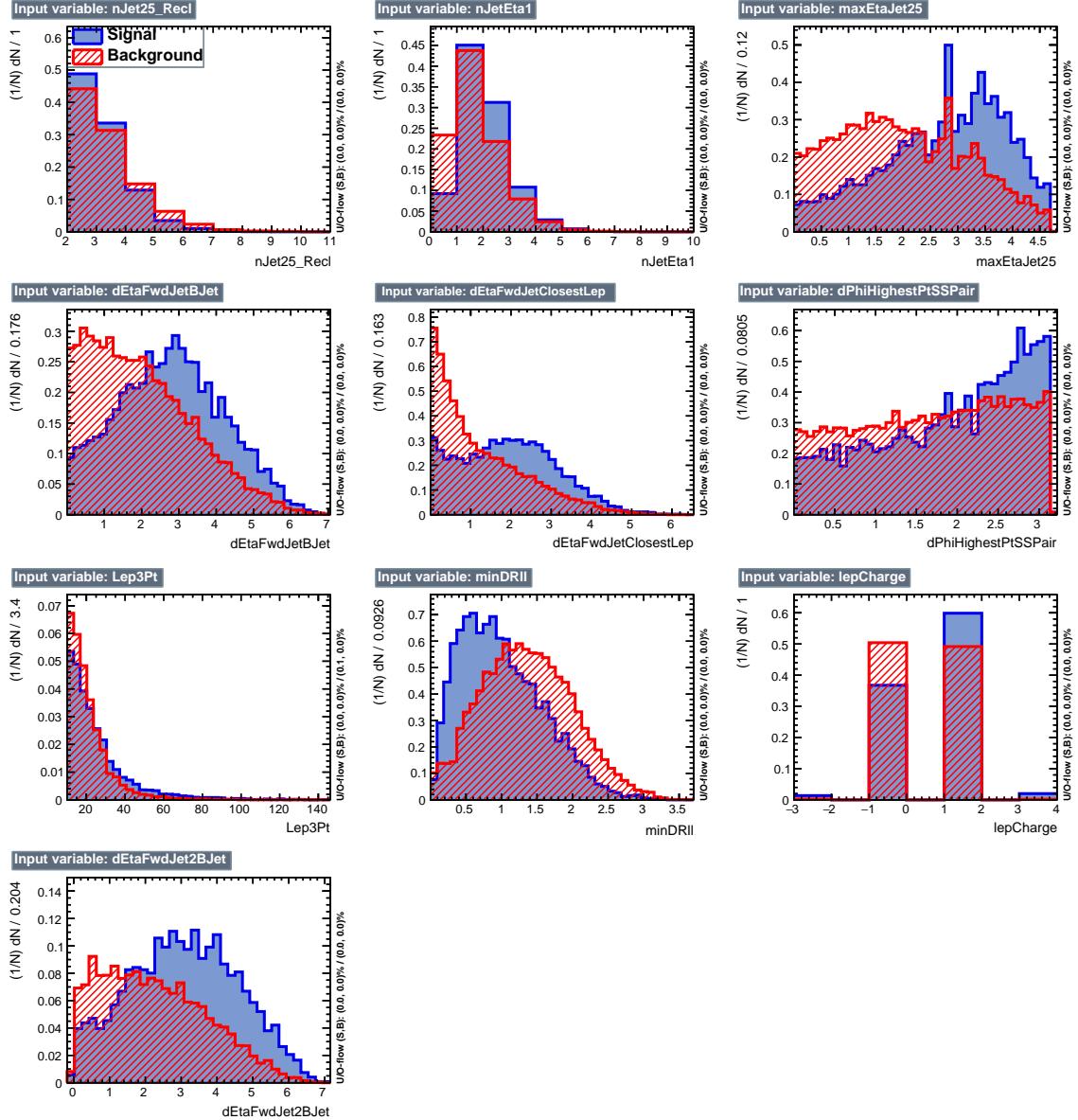


Figure B.7: BDT input variables as seen by BDTG classifier for the $3l$ channel, tHq signal (blue) discriminated against $t\bar{t}$ background (red).

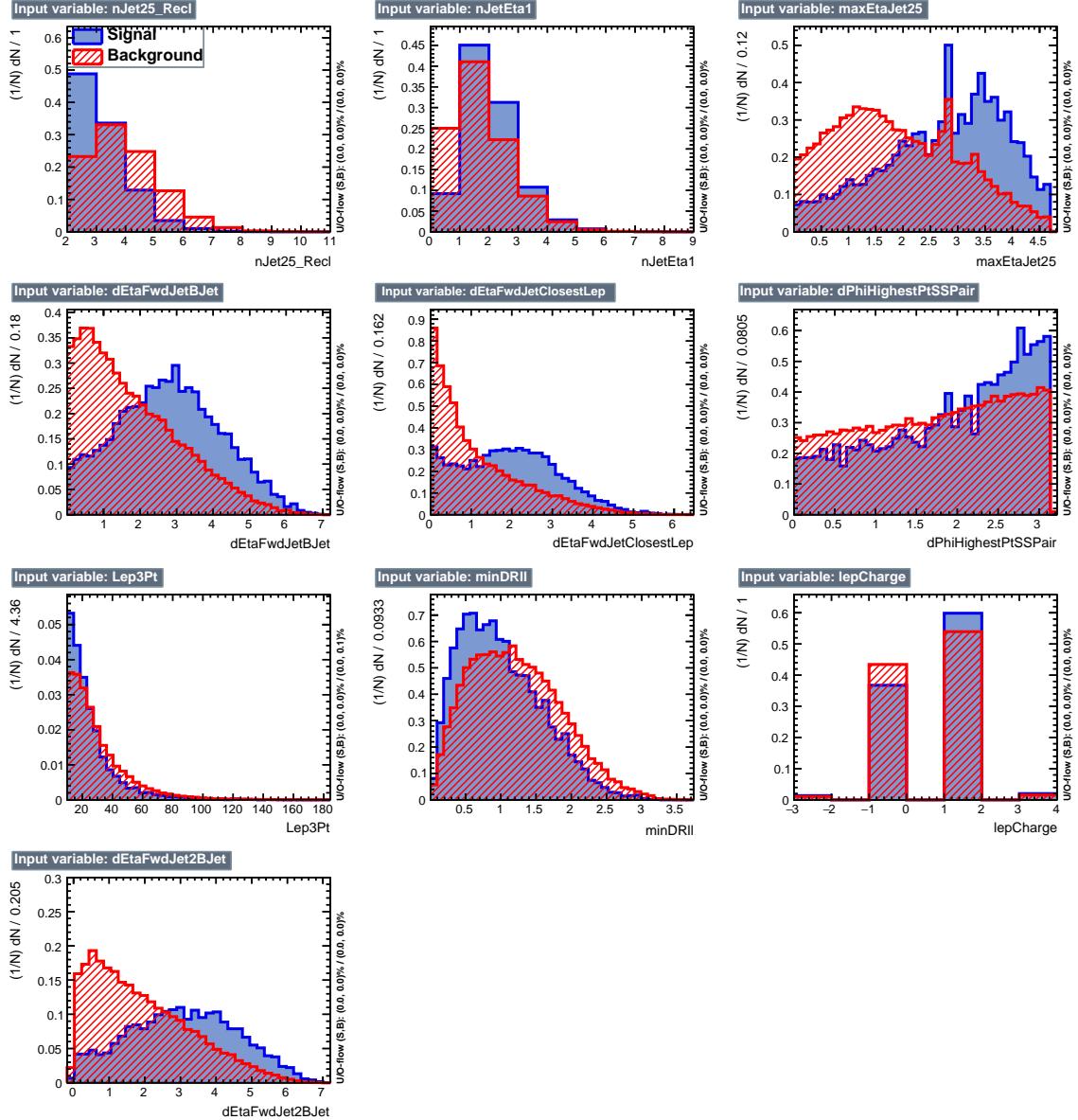


Figure B.8: BDT input variables as seen by BDTG classifier for the $3l$ channel, tHq signal (blue) discriminated against $t\bar{t}V$ background (red).

3272 **B.4 Pulls and impacts**

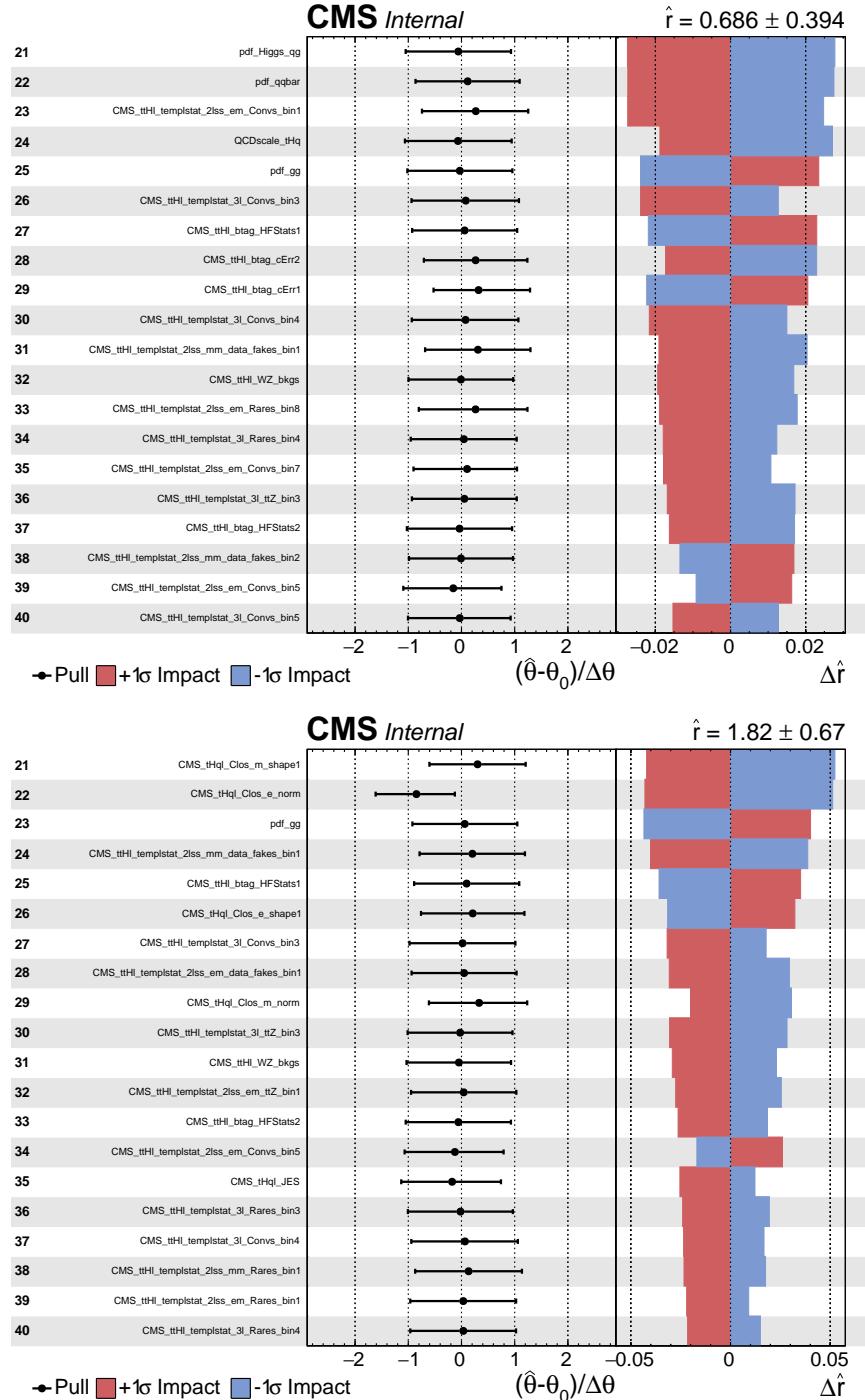


Figure B.9: Post-fit pulls and impacts of the next 20 nuisance parameters with largest impacts for the fit on the observed data, for the ITC (top) and SM (bottom) hypotheses.

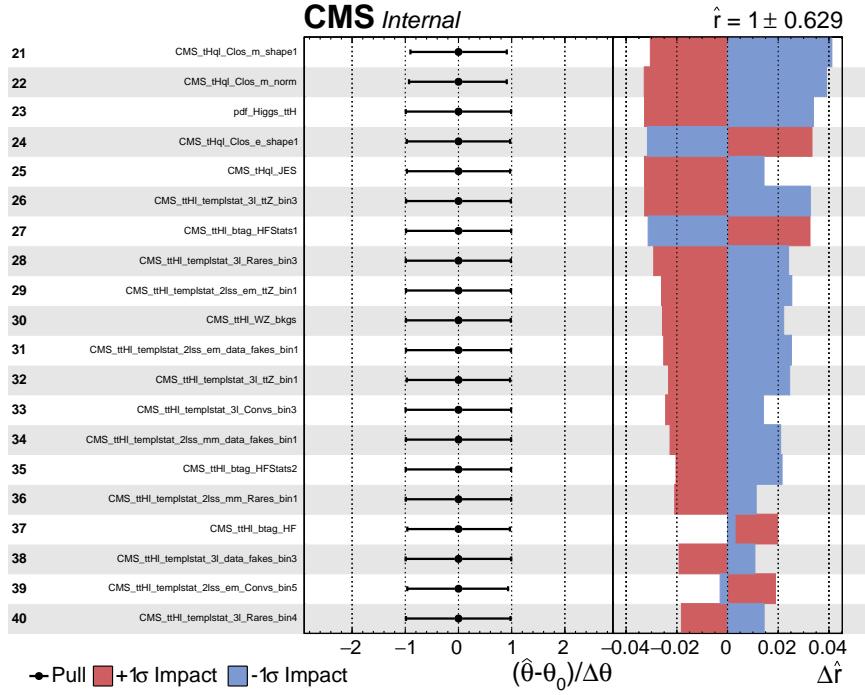


Figure B.10: Post-fit pulls and impacts of the next 20 nuisance parameters with largest impacts for a fit to the Asimov dataset with fixed signal strength, for the $\kappa_t/\kappa_V = -1.0$ hypothesis.

3273 **Appendix C**

3274 **Other binning strategies**

3275 Two additional strategies of clustering regions in the 2D plane of $BDTG_{tt}$ vs $BDTG_{ttV}$
3276 into bins were attempted, following studies done and documented in great detail in
3277 Reference [149]. A brief description is provided in the following.

3278 **Clustering by S/B ratio** In this method, the 2D plane is clustered into a given
3279 number of bins corresponding to regions where S/B is within a certain range. The
3280 bin borders are determined such that the number of background events in each bin is
3281 approximately equal. The resulting regions for $2lss$ and $3l$ events are shown in Figure
3282 C.1, while the expected distribution of signal and dominant backgrounds are shown
3283 in Figure C.2.

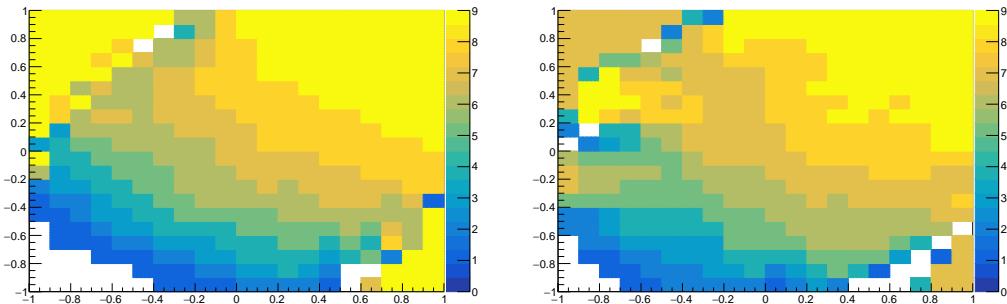


Figure C.1: Binning by S/B regions for $2lss$ (left) and $3l$ (right).

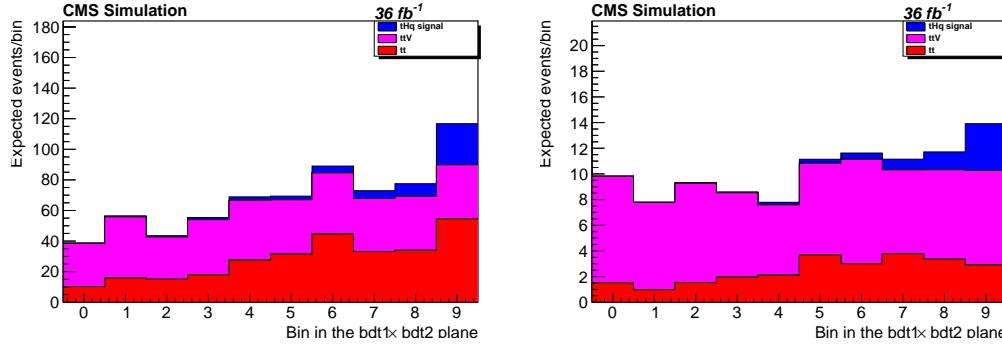


Figure C.2: Final bins (corresponding to S/B regions in the 2D plane) for $2lss$ and $3l$ (right).

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.

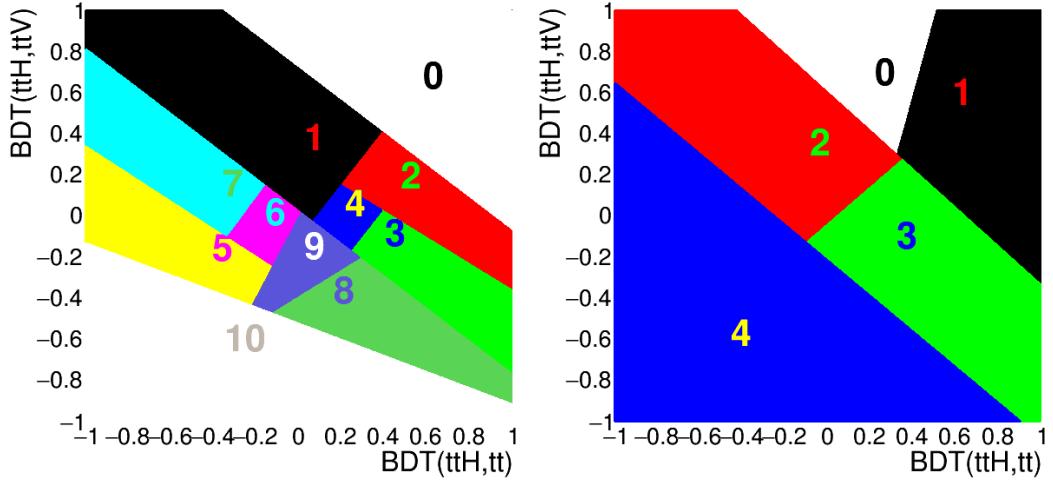


Figure C.3: Binning into geometric regions using a k -means algorithm for $2lss$ (left) and $3l$ (right).

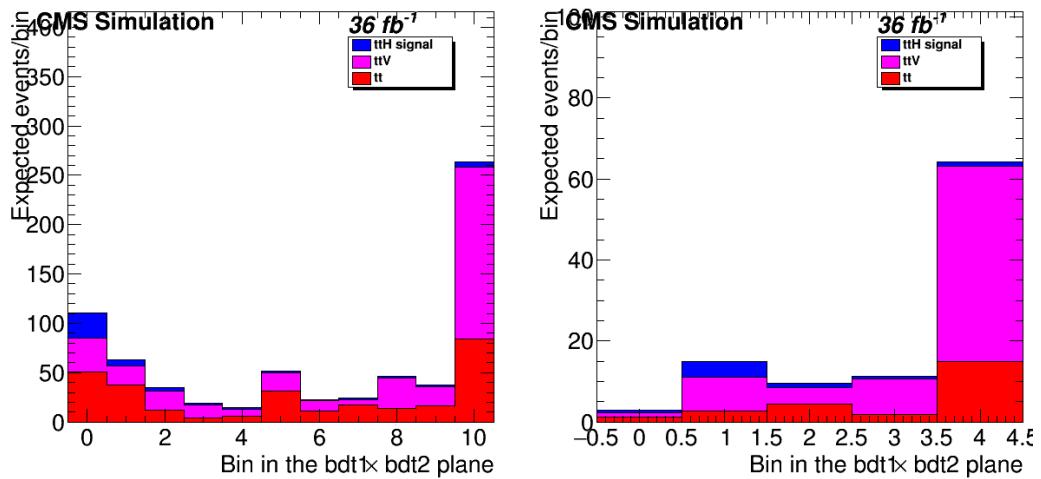


Figure C.4: Final bins using a k -means algorithm for $2lss$ (left) and $3l$ (right). Note that the bin numbering here is such that signal-like bins are lower.

³²⁹⁶ **Appendix D**

³²⁹⁷ **BDTG output variation with κ_V/κ_t**

³²⁹⁸ The BDTG classifier output was described in Section in the $\kappa_t = -1, \kappa_V = 1$ scenario;
³²⁹⁹ the change of BDTG classifiers output shape when varying the κ_V/κ_t coupling sce-
³³⁰⁰ nario is shown in Figure D.1 in the $3l$ channel for five different values of κ_t , with κ_V fixed at 1.0.

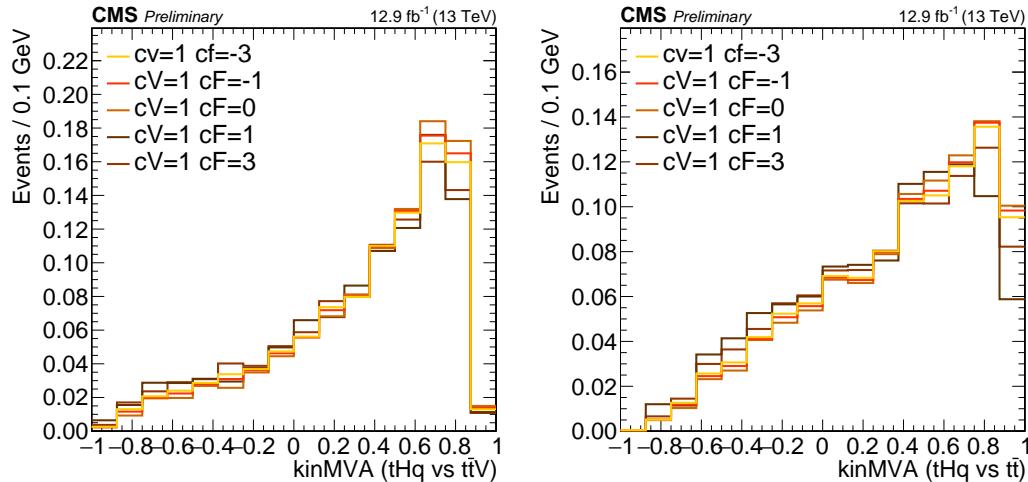


Figure D.1: Change of the BDTG classifiers output when varying κ_t coupling (κ_V is fixed at 1.0). Training vs. $t\bar{t}V$ (right) and vs. $t\bar{t}$ (left).

³³⁰¹

³³⁰² Complete this section !!!!!!! ask about this !

3303 **Appendix E**

3304 **tHq - $t\bar{t}H$ overlap**

3305 This section provides a quick overview of the differences and commonalities in event
3306 selections between this analysis and the $t\bar{t}H$ multilepton search [149]. The object
3307 selections of the two analysis are perfectly synchronized due to shared frameworks
3308 and samples. The only exception is the usage of forward jets ($|\eta| > 2.4, p_T > 40$ GeV)
3309 in this analysis. Such jets are not considered in the $t\bar{t}H$ analysis.

3310 Table E.1 gives an overview of the main differences in the event selections. Here,
3311 $E_T^{miss}_{LD}$ is defined as $E_T^{miss} \times 0.00397 + H_T^{miss} \times 0.00265$. Untagged jets in the tHq
3312 analysis are jets that do not pass the CSV loose working point and are either central
3313 ($|\eta| < 2.4, p_T > 25$ GeV) or forward ($|\eta| < 2.4, p_T > 40$ GeV). All jets in the $t\bar{t}H$ analysis
3314 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 $N_{jets}^{b, med.} \geq 1$ ≥ 1 un-tagged jet	Z veto, 10 GeV $N_{jets}^{b, med.} \geq 1$ OR $N_{jets}^{b, loose} \geq 2$ $E_T^{miss}_{LD} > 0.2$ OR $N_{jets}^{centr.} \geq 4$
2lss	$N_{jets}^{b, med.} \geq 1$ ≥ 1 un-tagged jet	$N_{jets}^{b, med.} \geq 1$ OR $N_{jets}^{b, loose} \geq 2$ $N_{jets}^{central} \geq 4$

Table E.1: Differences in event selection between this analysis and the $t\bar{t}H$ multilepton analysis.

3315 Table E.2 shows the total events yields in the individual channels, and the yield
 3316 of shared events between each channel, for the tHq signal sample, the $t\bar{t}H$ signal
 3317 sample, and the data. In the data, for the $3l$ channel, about 80% of events passing
 3318 the tHq selection also pass the $t\bar{t}H$ selection, constituting about 70% of that channel.
 3319 In the $2lss$ channel, about 50% of data events passing the tHq selection also pass the
 3320 $t\bar{t}H$ selection, but these events constitute almost 90% of the $t\bar{t}H$ selection in those
 3321 channels. Similar overlaps are also seen in the tHq and $t\bar{t}H$ signal samples.

3322 There is no migration between different channels and different selections, i.e. no
 3323 events passing the selection of a given tHq channel pass the selection of any other
 3324 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.

3325 **Appendix F**

3326 **Forward jet impact plots**

3327 The impact of the data/MC disagreement for forward jet η is observed to reduce with
3328 higher p_T cuts; Figures F.1, F.2 and F.3 show this reduction in the impact of the
3329 forward jet η nuisance in the fit.

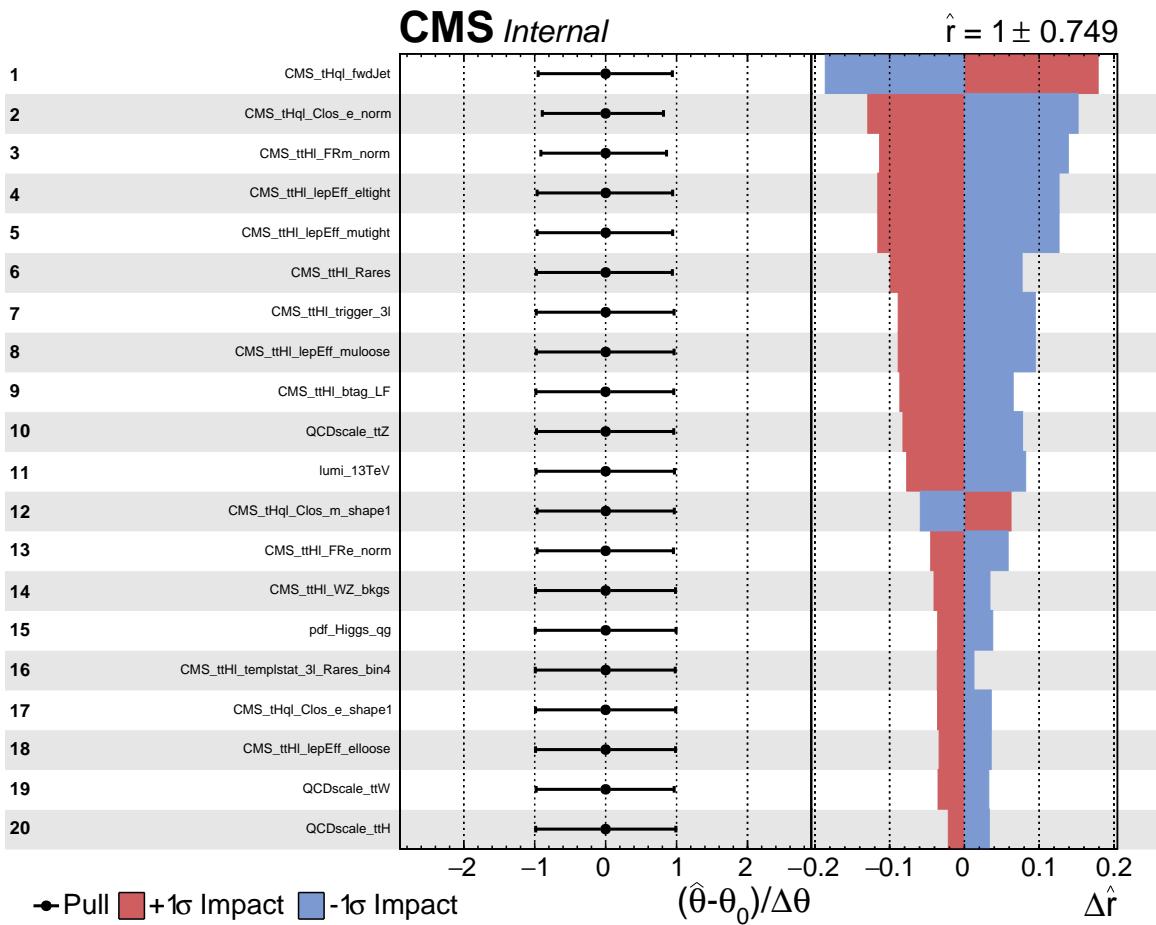


Figure F.1: Post-fit pulls and impacts of the 20 nuisance parameters with p_T cut 25 GeV for the forward jet.

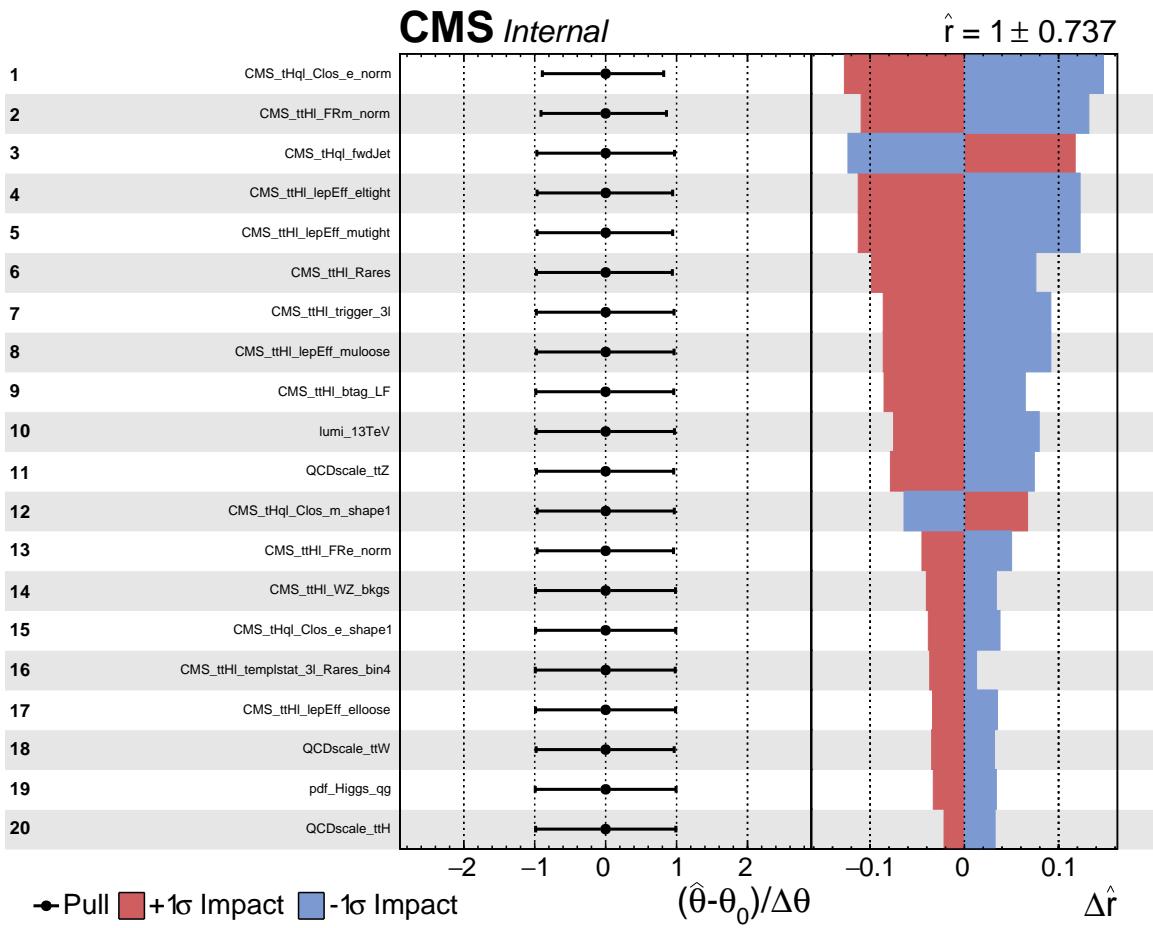


Figure F.2: Post-fit pulls and impacts of the 20 nuisance parameters with p_T cut 30 GeV for the forward jet.

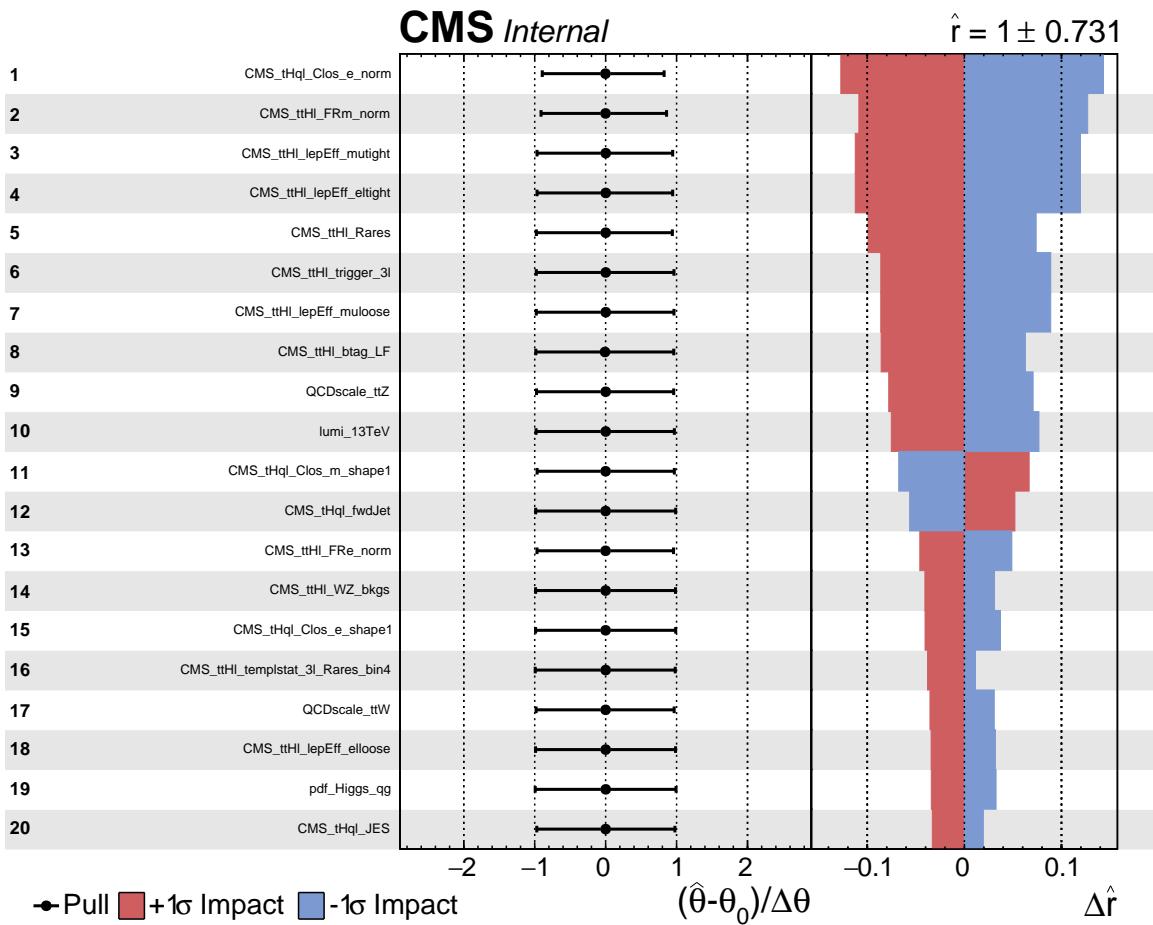


Figure F.3: Post-fit pulls and impacts of the 20 nuisance parameters with p_T cut 40 GeV for the forward jet.

₃₃₃₀ **Appendix G**

₃₃₃₁ **Cross sections and Branching**

₃₃₃₂ **ratios scalings**

κ_V	κ_t	HWW	HZZ	H $\tau\tau$	H $\mu\mu$	Hbb	Hcc	H $\gamma\gamma$	HZ γ	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. κ_t and $\kappa_V = 0.5$ for the non-resolved model.

κ_V	κ_t	HWW	HZZ	H $\tau\tau$	H $\mu\mu$	Hbb	Hcc	H $\gamma\gamma$	HZ γ	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. κ_t and $\kappa_V = 1.0$ for the non-resolved model.

κ_V	κ_t	HWW	HZZ	H $\tau\tau$	H $\mu\mu$	Hbb	Hcc	H $\gamma\gamma$	HZ γ	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. κ_t and $\kappa_V = 1.5$ for the non-resolved model.

κ_V	κ_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 $\kappa_V = 0.5$.

κ_V	κ_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 $\kappa_V = 1.0$.

κ_V	κ_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 $\kappa_V = 1.5$.

$\cos(\alpha_{CP})$	Cross section (pb)			95% C.L. Limits		Cross section limits (pb)	
	tHq	tHW	$t\bar{t}H$	Exp.	Obs.	Exp.	Obs.
-1.0	$0.794^{+2.8}_{-4.0}$	$0.146^{+0.2}_{-0.2}$	0.503436	$0.691^{+0.204}_{-0.299}$	1.489	$0.302^{+0.089}_{-0.131}$	0.651
-0.9	$0.728^{+2.7}_{-4.1}$	$0.135^{+0.2}_{-0.2}$	0.426117	$0.768^{+0.228}_{-0.333}$	1.632	$0.300^{+0.089}_{-0.130}$	0.637
-0.8	$0.664^{+2.7}_{-4.2}$	$0.123^{+0.2}_{-0.2}$	0.355670	$0.860^{+0.256}_{-0.374}$	1.797	$0.298^{+0.088}_{-0.130}$	0.622
-0.7	$0.601^{+2.8}_{-4.0}$	$0.112^{+0.2}_{-0.2}$	0.295533	$0.965^{+0.287}_{-0.423}$	1.984	$0.295^{+0.088}_{-0.129}$	0.606
-0.6	$0.546^{+2.9}_{-4.3}$	$0.102^{+0.2}_{-0.2}$	0.242268	$1.082^{+0.323}_{-0.476}$	2.172	$0.292^{+0.087}_{-0.128}$	0.586
-0.5	$0.497^{+3.1}_{-4.2}$	$0.092^{+0.2}_{-0.2}$	0.197595	$1.209^{+0.362}_{-0.534}$	2.362	$0.288^{+0.086}_{-0.127}$	0.563
-0.4	$0.446^{+3.1}_{-4.5}$	$0.083^{+0.2}_{-0.2}$	0.159794	$1.362^{+0.409}_{-0.605}$	2.595	$0.284^{+0.085}_{-0.126}$	0.542
-0.3	$0.398^{+3.2}_{-4.6}$	$0.074^{+0.2}_{-0.2}$	0.132302	$1.538^{+0.463}_{-0.684}$	2.870	$0.282^{+0.085}_{-0.125}$	0.526
-0.2	$0.353^{+3.5}_{-4.8}$	$0.066^{+0.2}_{-0.2}$	0.111684	$1.739^{+0.524}_{-0.776}$	3.205	$0.280^{+0.084}_{-0.125}$	0.515
-0.1	$0.314^{+3.7}_{-4.9}$	$0.059^{+0.2}_{-0.2}$	0.099656	$1.952^{+0.588}_{-0.870}$	3.597	$0.280^{+0.084}_{-0.125}$	0.515
0.0	$0.275^{+3.6}_{-5.2}$	$0.052^{+0.2}_{-0.2}$	0.094502	$2.208^{+0.664}_{-0.982}$	4.149	$0.282^{+0.085}_{-0.125}$	0.530
0.1	$0.242^{+4.0}_{-5.5}$	$0.045^{+0.2}_{-0.2}$	0.099656	$2.458^{+0.737}_{-0.889}$	4.822	$0.288^{+0.086}_{-0.128}$	0.565
0.2	$0.211^{+4.1}_{-5.8}$	$0.040^{+0.2}_{-0.2}$	0.111684	$2.690^{+0.801}_{-0.178}$	5.583	$0.296^{+0.088}_{-0.129}$	0.613
0.3	$0.182^{+4.1}_{-6.1}$	$0.035^{+0.2}_{-0.2}$	0.132302	$2.856^{+0.842}_{-0.234}$	6.242	$0.302^{+0.089}_{-0.131}$	0.661
0.4	$0.156^{+4.4}_{-6.5}$	$0.030^{+0.2}_{-0.2}$	0.159794	$2.898^{+0.845}_{-0.235}$	6.536	$0.304^{+0.089}_{-0.129}$	0.685
0.5	$0.134^{+4.5}_{-6.6}$	$0.026^{+0.2}_{-0.2}$	0.197595	$2.739^{+0.793}_{-0.157}$	6.281	$0.297^{+0.086}_{-0.125}$	0.681
0.6	$0.116^{+4.7}_{-6.9}$	$0.023^{+0.2}_{-0.2}$	0.242268	$2.460^{+0.710}_{-0.038}$	5.692	$0.284^{+0.082}_{-0.120}$	0.658
0.7	$0.100^{+5.0}_{-7.1}$	$0.020^{+0.2}_{-0.2}$	0.295533	$2.138^{+0.617}_{-0.904}$	4.971	$0.269^{+0.078}_{-0.114}$	0.626
0.8	$0.087^{+4.8}_{-7.1}$	$0.018^{+0.2}_{-0.2}$	0.357388	$1.830^{+0.528}_{-0.776}$	4.263	$0.256^{+0.074}_{-0.109}$	0.597
0.9	$0.077^{+4.7}_{-7.0}$	$0.017^{+0.2}_{-0.2}$	0.426117	$1.549^{+0.448}_{-0.658}$	3.610	$0.244^{+0.071}_{-0.104}$	0.569
1.0	$0.071^{+4.2}_{-6.7}$	$0.016^{+0.2}_{-0.2}$	0.503436	$1.322^{+0.383}_{-0.562}$	3.080	$0.236^{+0.068}_{-0.100}$	0.551

Table G.7: Production cross sections for tHq , tHW and $t\bar{t}H$ at $\sqrt{s} = 13$ TeV, as a function of $\cos(\alpha_{CP})$. The quoted uncertainties on the cross section correspond to scale variations in %. The used $t\bar{t}H$ NLO cross sections are obtained from [47] and are interpolated to the angles for which the LHE weights in the signal MC samples are available. Also listed are the expected and observed asymptotic limits at 95% C.L. for all studied CP-mixing angles. The uncertainties on the expected limit correspond to $\pm 1\sigma$.

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