$HH \to b\bar{b}b\bar{b}$ or How I Learned to Stop Worrying and Love the QCD Background

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A dissertation
submitted in partial fulfillment of the
requirements for the degree of

Doctor of Philosophy

University of Washington

2021

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Abstract

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Physics

Insert abstract here

TABLE OF CONTENTS

LIST OF FIGURES

GLOSSARY

ARGUMENT: replacement text which customizes a L*A*T*E*X macro for each particular usage.

ACKNOWLEDGMENTS

As anyone who has written a Ph.D. thesis will probably tell you, it's been a journey. We laughed, we cried, we bled occasionally (though nothing too serious). A pandemic happened, I learned how to make sourdough (see the appendix for more details). I learned how to ski, discovered a love for hiking, and ate large amounts of cheese. The list of people who I have met and shared deep and memorable experiences with is long – I fear to list you all here in case I miss someone! – but please do know that I treasure you. This is the beauty and tragedy of doing a Ph.D. half in Seattle, half at CERN: it allows you to build strong friendships with a large group of people, and then scatters you all across the globe. So to the Seattle friends, to the CERN friends, to the friends from undergrad, and high school, and even earlier, and to everyone in between, thank you for being a part of my life, and I hope to see you soon.

Of course, a thank you to my family for their continuing support, vacationing adventures, and for trying their best to learn physics along with me (my dad re: ATLAS – "This is pretty complicated isn't it?").

And finally a huge thank you to my group: Anna, for your guidance and support, and for always caring about me as a person in addition to me as a physicist. And Jana, for guidance and support, of course, but also for looking at/giving comments on almost literally every single one of my talks (even if you didn't always get my jokes).

DEDICATION

To life!

Chapter 1

THE STANDARD MODEL OF PARTICLE PHYSICS

"I may be bad, but I'm perfectly good at it" - Rihanna re: the Standard Model (SM), or so I've been told

The Standard Model of Particle Physics (SM) is a monumental historical achievement, providing a formalism with which one may describe everything from the physics of everyday experience to the physics that is studied at very high energies at the Large Hadron Collider (Chapter 3). In this chapter, we will provide a brief overview of the pieces that go into the construction of such a model. The primary focus of this thesis is searches for pair production of Higgs bosons decaying to four b-quarks. Consequently, we will pay particular attention to the relevant pieces of the Higgs Mechanism, as well as the theory behind searches at a hadronic collider.

1.1 Introduction: Particles and Fields

What is a particle? The Standard Model describes a set of fundamental, point-like, objects (shown in Figure SM FIGURE). These objects have distinguishing characteristics (e.g., mass and spin). These objects interact in very specific ways. The set of objects and their interactions result in a set of observable effects, and these effects are the basis of a field of experimental physics.

The effects of these objects and their interactions are familiar as fundamental forces: electromagnetism (photons, electrons), the strong interaction (quarks, gluons), the weak interaction (neutrinos, W and Z bosons). Gravity is not described in this model, as the

weakest, with effects most relevant on much larger distance scales than the rest. However, the description of these other three is powerful – verifying and searching for cracks in this description is a large effort, and the topic of this thesis.

The formalism for describing these particles and their interactions is that of quantum field theory. Classical field theory is most familiar in the context of, e.g., electromagnetism – an electric field exists in some region of space, and a charged point-particle experiences a force characterized by the charge of the point-particle and the magnitude of the field at the location of the point-particle in spacetime. The same language translates to quantum field theory. Here, particles are described in terms of quantum fields in some region of spacetime. These fields have associated charges which describe the forces they experience when interacting with other quantum fields. Most familiar is electric charge – however this applies to e.g., the strong interaction as well, where quantum fields have an associated *color charge* describing behavior under the strong force.

Particles are observed to behave in different ways under different forces. These behaviors respect certain *symmetries*, which are most naturally described in the language of group theory. The respective fields, charges, and generators of these symmetry groups are the basic pieces of the SM Lagrangian, which describes the full dynamics of the theory. In the following, we will build up the basic components of this Lagrangian.

1.2 Quantum Electrodynamics

Classical electrodynamics is familiar to the general physics audience: electric $(\vec{E})$ and magnetic $(\vec{B})$ fields are used to describe behavior of particles with charge q moving with velocity $\vec{v}$, with forces described as $\vec{F} = q\vec{E} + q\vec{v} \times \vec{B}$. Hints at some more fundamental properties of electric and magnetic fields come via a simple thought experiment: in a frame of reference moving along with the particle at velocity $\vec{v}$, the particle would appear to be standing still, and therefore have no magnetic force exerted. Therefore a *relativistic* formulation of the theory is required. This is most easily accomplished with a repackaging: the fundamental objects are

no longer classical fields but the electric and magnetic *potentials*: ϕ and $\vec{A}$ respectively, with

$$\vec{E} = -\boldsymbol{\nabla}\phi - \frac{\partial \vec{A}}{\partial t} \tag{1.1}$$

$$\vec{B} = \boldsymbol{\nabla} \times \vec{A} \tag{1.2}$$

It is then natural to fully repackage into a relativistic *four-vector*: $A_\mu = (\phi, \vec{A})$. Considering $\partial^\mu = (\frac{\partial}{\partial t}, \boldsymbol{\nabla})$, the x components of these above two equations become: *TODO: Check signs and units!! Add Jackson reference?*

$$E_x = -\frac{\partial \phi}{\partial x} + \frac{\partial A_x}{\partial t} = (\partial^0 A^1 - \partial^1 A^0) \tag{1.3}$$

$$B_x = \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} = (\partial^2 A^3 - \partial^3 A^2) \tag{1.4}$$

This is naturally suggestive of a second rank, antisymmetric tensor to describe both the electric and magnetic fields (the *field strength tensor*), defined as:

$$F^{\alpha\beta} = \partial^\alpha A^\beta - \partial^\beta A^\alpha \tag{1.5}$$

Defining a four-current as $J_\mu = (q, \vec{J})$, with q standard electric charge, $\vec{J}$ standard electric current, conservation of charge may be expressed via the continuity equation

$$\partial_\mu J^\mu = 0 \tag{1.6}$$

and all of classical electromagnetism may be packaged into the Lagrangian density:

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - J^\mu A_\mu. \tag{1.7}$$

This gets us partway to our goal, but is entirely classical - the description is of classical fields and point charges, not of quantum fields and particles. To reframe this, let us go back to the zoomed out view of the particles of the Standard Model. Two of the most familiar objects associated with electromagnetism are electrons: spin-1/2 particles with charge e, mass m, and photons: massless spin-1 particles which are the "pieces" of electromagnetic radiation.

We know that electrons experience electromagnetic interactions with other objects. Given this, and the fact that such interactions must be transmitted *somehow* between e.g. two

electrons, it seems natural that these interactions are facilitated by electromagnetic radiation. More specifically, we may think of photons as *mediators* of the electromagnetic force. It follows, then, that a description of electromagnetism on the level of particles must involve a description of both the "source" particles (e.g. electrons), the mediators (photons), and their interactions. Further, this description must be (1) relativistic and (2) consistent with the classically derived dynamics described above.

The beginnings of a relativistic description of spin-1/2 particles is due to Paul Dirac, with the famous Dirac equation:

$$(i\gamma^\mu \partial_\mu - m)\psi = 0 \tag{1.8}$$

where ∂_μ is as defined above, ψ is a Dirac *spinor*, i.e. a four-component wavefunction, m is the mass of the particle, and γ^μ are the Dirac gamma matrices, which define the algebraic structure of the theory.

TODO: Add some stuff about the conjugate?

The Dirac equation is the dynamical equation for spin-1/2, but we'd like to express these dynamics via a Lagrangian density. Further, to have a relativistic description, we'd like to have this be density be Lorentz invariant. These constraints lead to a Lagrangian of the form

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi \tag{1.9}$$

where the Euler-Lagrange equation exactly recovers the Dirac equation.

The question now becomes how to marry the two Lagrangian descriptions that we have developed. Returning for a moment to classical electrodynamics, we know that the Hamiltonian for a charged particle in an electromagnetic field is described by

$$H = \frac{1}{2m}(\vec{p} - q\vec{A})^2 + q\phi. \tag{1.10}$$

Comparing this to the Hamiltonian for a free particle, we see that the modifications required are $\vec{p} \to \vec{p} - q\vec{A}$ and $E \to E - q\phi$. Using the canonical quantization trick of identifying $\vec{p}$ with operator $-i\nabla$ and E with operator $i\frac{\partial}{\partial t}$, this identification becomes

$$i\partial_\mu \to i\partial_\mu - qA_\mu \tag{1.11}$$

Allowing for the naive substitution in the Dirac Lagrangian *TODO: Source term?*:

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu(\partial_\mu + iqA_\mu) - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \tag{1.12}$$

Setting $q = e$ here (as appropriate for the case of an electron), and defining $D_\mu \equiv \partial_\mu + ieA_\mu$, this may then be written in the form

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \tag{1.13}$$

which is exactly the quantum electrodynamics Lagrangian.

We have swept a few things under the rug here, however. Recall that the general form of a Lagrangian is conventionally $\mathcal{L} = T - V$, where T is the kinetic term, and thus ought to contain a derivative with respect to time (c.f. the standard $\frac{1}{2}m\frac{\partial x}{\partial t}$ familiar from basic kinematics). More particularly, given the definition of conjugate momentum as $\partial\mathcal{L}/\partial\dot{q}$ for $\mathcal{L}(q, \dot{q}, t)$ and $\dot{q} = \frac{\partial q}{\partial t}$, any field q which has no time derivative in the Lagrangian has 0 conjugate momentum, and thus no dynamics.

Looking at this final form, there is an easily identifiable kinetic term for the spinor fields (just applying the D_μ operator). However trying to identify something similar for the A fields, one comes up short – the antisymmetric nature of $F^{\mu\nu}$ term means that there is no time derivative applied to A^0.

What does this mean? A^μ is a four component object, but it would appear that only three of the components have dynamics: we have too many degrees of freedom in the theory. This is the principle behind *gauge symmetry* – an extra constraint on A^μ (a *gauge condition*) must be defined such that a unique A^μ defines the theory and satisfies the condition. However, we are free to choose this extra condition – the physics content of the theory should be independent of this choice (that is, it should be *gauge invariant*).

To ground this a bit, let us return to basic electric and magnetic fields. These are physical quantities that can be measured, and are defined in terms of potentials as

$$\vec{E} = -\boldsymbol{\nabla}\phi - \frac{\partial\vec{A}}{\partial t} \tag{1.14}$$

$$\vec{B} = \boldsymbol{\nabla} \times \vec{A}. \tag{1.15}$$

It is easy to show, for any scalar function λ, that $\boldsymbol{\nabla} \times \boldsymbol{\nabla}\lambda = 0$. This implies that the physical $\vec{B}$ field is invariant under the transformation $\vec{A} \to \vec{A} + \boldsymbol{\nabla}\lambda$ for any scalar function λ.

Under the same transformation of $\vec{A}$, the electric field $\vec{E}$ becomes $-\boldsymbol{\nabla}\phi - \frac{\partial \vec{A}}{\partial t} - \frac{\partial \boldsymbol{\nabla}\lambda}{\partial t} = -\boldsymbol{\nabla}\left(\phi + \frac{\partial \lambda}{\partial t}\right) - \frac{\partial \vec{A}}{\partial t}$, such that, for the $\vec{E}$ field to be unchanged, we must additionally apply the transformation $\phi \to \phi - \frac{\partial \lambda}{\partial t}$.

TODO: Check signs here too! This is set of transformations to the potentials that leave the physical degrees of freedom invariant is expressed in our four vector notation naturally as

$$A_\mu \to A_\mu - \partial_\mu \lambda \tag{1.16}$$

where $A_\mu = (\phi, -\vec{A})$ with our sign convention. It should be noted that this function λ is an arbitrary function of *local* spacetime, and thus expresses invariance of the physics content under a local transformation.

Let us return to the Lagrangian for QED. In particular, focusing on the free Dirac piece

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi \tag{1.17}$$

we note that if we apply a local transformation of the form $\psi \to e^{iq\lambda(x)}\psi$ (and correspondingly $\bar{\psi} \to \bar{\psi}e^{-iq\lambda(x)}$, by definition), the Lagrangian becomes

$$\bar{\psi}e^{-iq\lambda(x)}(i\gamma^\mu \partial_\mu - m)e^{iq\lambda(x)}\psi = \bar{\psi}e^{-iq\lambda(x)}(i\gamma^\mu \partial_\mu)e^{iq\lambda(x)}\psi - m\bar{\psi}\psi. \tag{1.18}$$

As $\partial_\mu(e^{iq\lambda(x)}\psi) = iqe^{iq\lambda(x)}(\partial_\mu\lambda(x))\psi + e^{iq\lambda(x)}\partial_\mu\psi$, this becomes

$$\bar{\psi}(i\gamma^\mu(\partial_\mu + iq\partial_\mu\lambda(x)) - m)\psi. \tag{1.19}$$

Thus, the free Dirac Lagrangian on its own is not invariant under this transformation. We may note, however, that on interaction with an electromagntic field, as described above, this transformed Lagrangian may be packaged as:

$$\bar{\psi}(i\gamma^\mu(\partial_\mu + iq\partial_\mu\lambda(x) + iqA_\mu) - m)\psi = \bar{\psi}(i\gamma^\mu(\partial_\mu + iq(A_\mu + \partial_\mu\lambda(x)) - m)\psi. \tag{1.20}$$

since by the arguments above, the physics content of the Lagrangian is invariant under the transformation $A_\mu \to A_\mu - \partial_\mu\lambda$, we may directly make this transformation, and remove this

extra $\partial_\mu\lambda(x)$ term. It is straightforward to verify that the $\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$ term is invariant under this same transformation of A_μ, so we may say that the QED Lagrangian is invariant under local transformations of the form $\psi \to e^{iq\lambda(x)}\psi$.

These arguments illuminate some important concepts which will serve us well going forward. First, while we have remained grounded in the "familiar" physics of electromagnetism for the above, arguments of the "top down" variety would lead us to the exact same conclusions. That is, suppose we wanted to construct a theory of spin-1/2 particles that was invariant under local transformations of the form $\psi \to e^{iq\lambda(x)}\psi$. More broadly, we could say that we desire this theory to be invariant under local $U(1)$ transformations, where $U(1)$ is exactly this group, under multiplication, of complex numbers with absolute value 1. By very similar arguments as above, we would see that, to achieve invariance, this theory would necessitate an additional degree of freedom, A_μ, with the exact properties that are familiar to us from electrodynamics. These arguments based on symmetries are extremely powerful in building theories with a less familiar grounding, as we will see in the following.

Second, we defined this quantity $D_\mu \equiv \partial_\mu + ieA_\mu$ above, seemingly as a matter of notational convenience. However, from the latter set of arguments, such a packaging takes on a new power: by explicitly including this gauge field A_μ which transforms in such a way as to keep invariance under a given transformation, the invariance is immediately more manifest. That is, to pose the $U(1)$ invariance in a more zoomed out way, under the transformation $\psi \to e^{iq\lambda(x)}\psi$, while

$$\bar{\psi}\partial_\mu\psi \to \bar{\psi}(\partial_\mu + iq\partial_\mu\lambda(x))\psi \tag{1.21}$$

with the extra term that gets canceled out by the gauge transformation of A_μ,

$$\bar{\psi}D_\mu\psi \to \bar{\psi}D_\mu\psi \tag{1.22}$$

where this transformation is already folded in. This repackaging, called a *gauge covariant derivative* is much more immediately expressive of the symmetries of the theory.

Finally, to emphasize how fundamental these gauge symmetries are to the corresponding theory, let us examine the additional term needed for $U(1)$ invariance, $q\bar{\psi}\gamma^\mu A_\mu\psi$. While a

first principles examination of Feynman rules is beyond the scope of this thesis, it is powerful to note that this is expressive of a QED vertex: the $U(1)$ invariance of the theory and the interaction between photons and electrons are inextricably tied together.

1.3 An Aside on Group Theory

TODO: word on exponential representation? Quantum electrodynamics is very familiar and well covered, and provides (both historically and in this thesis) a nice bridge between "standard" physics and the language of symmetries and quantum field theory. However, now that we are acquainted with the language, we may set up to dive a bit deeper. To begin, let us look again at the $U(1)$ group that is so fundamental to QED. We have expressed this via a set of transformations on our Dirac spinor objects, ψ, of the form $e^{iq\lambda(x)}$. Note that such transformations, though they are local (i.e. a function of spacetime) are purely *phase* transformations. Relatedly, $U(1)$ is an Abelian group, meaning that group elements commute.

To set up language to generalize beyond $U(1)$, note that we may equivalently write $U(1)$ elements as $e^{ig\vec{\alpha}(x)\cdot\vec{T}}$, $\vec{\alpha}(x)$ and $\vec{T}$ and are vectors in the space of *generators* of the group, with each $\alpha^a(x)$ an associated scalar function to generator t^a, and g is some scalar strength parameter. Of course this is a bit silly for $U(1)$, which has a single generator, and thus reduces to the transformation we discussed above. However, this becomes much more useful for groups of higher degree, with more generators and degrees of freedom.

To discuss these groups in a bit more detail, note that $U(n)$ is the unitary group of degree n, and corresponds to the group of $n \times n$ unitary matrices (that is, $U^\dagger U = U U^\dagger = 1$). Given that group elements are $n \times n$, this means that there are n^2 degrees of freedom: n^2 generators are needed to characterize the group.

For $U(1)$, this is all consistent with what we have said above – the group of 1×1 unitary matrices have a single generator, and the phases we identify above clearly satisfy unitarity. Note that these degrees of freedom for the gauge group also characterize the number of gauge bosons we need to satisfy the local symmetry: for $U(1)$, we need one gauge boson, the photon.

Of relevance for the Standard Model are also the special unitary groups $SU(n)$. These

are defined similarly to the unitary groups, with the additional requirement that group elements have determinant 1. This extra constraint removes 1 degree of freedom: groups are characterized by $n^2 - 1$ generators.

In particular, we will examine the groups $SU(2)$ in the context of the weak interaction, with an associated $2^2 - 1 = 3$ gauge bosons (cf. the $W^{\pm}$ and Z bosons), and $SU(3)$, with an associated $3^2 - 1 = 8$ gauge bosons (cf. gluons of different flavors). Note that these groups are non-Abelian (2×2 or 3×3 matrices do not, in general, commute), leading to a variety of complications. However, both of these theories feature interactions with spin-1/2 particles, with transformations of a very similar form: $\psi \to e^{ig\vec{\alpha}(x) \cdot \vec{T}} \psi$, and the general framing of the arguments for QED will serve us well in the following.

1.4 Quantum Chromodynamics

In some sense, the simplest extension the development of QED is quantum chromodynamics (QCD). QCD is a theory in which, once the basic dynamics are framed (a non-trivial task!) the group structure becomes apparent. The quark model, developed by Murray Gell-Mann and George Zweig*TODO: cite*, provided the fundamental particles involved in the theory, and had great success in explaining the expanding zoo of experimentally observed hadronic states.

Some puzzles were still apparent – the Δ^{++} baryon, e.g., is composed of three up quarks, u, with aligned spins. As quarks are fermions, such a state should not be allowed by the Pauli exclusion principle. The existence of such a state in nature implies the existence of another quantum number, and a triplet of values, called *color charge* was proposed by Oscar Greenburg *TODO: cite*. With these pieces in place, the structure becomes more apparent, as elucidated by Han and Nambu *TODO: cite: https://digital.library.unt.edu/ark:/67531/metadc1031342/m1/6/*.

Let us reason our way to the symmetries using color charge. Experimentally, we know that there is this triplet of color charge values r, g, b (the "plus" values, cf. electric charge) and correspondingly anti-color charge $\bar{r}, \bar{g}, \bar{b}$ (the "minus" values). Supposing that the force behind QCD (the *strong force*) is, similar to QED, interactions between fermions mediated by gauge bosons (quarks and gluons respectively), we can start to line up the pieces.

What color charge does a gluon have? Similarly to electric charge, we may associate particles with color charge, anti-particles with anti-color charge. Notably, free particles observed experimentally are colorless (have no color charge). Thus, in order for charge to be conserved throughout such processes, this already implies that there are charged gluons. Further, examining color flow diagrams such as *TODO: insert*, it is apparent first that a gluon has not one but two associated color charges and second that these two must be one color charge and one anti-color charge.

Counting up the available types of gluons, then, we come up with nine. Six of mixed color type: $r\bar{b}, r\bar{g}, b\bar{r}, b\bar{g}, g\bar{b}$, and $g\bar{r}$, and three of same color type: $r\bar{r}$, $g\bar{g}$, and $b\bar{b}$. In practice, however, these latter three are a bit redundant: all express a colorless gluon, which, if we could observe this as a free particle, would be indistinguishable from each other. The *color singlet* state is then a mix of these, $\frac{1}{\sqrt{3}}(r\bar{r} + g\bar{g} + b\bar{b})$, leaving two unclaimed degrees of freedom, which may be satisfied by the linearly independent combinations $\frac{1}{\sqrt{2}}(r\bar{r} - g\bar{g})$ and $\frac{1}{\sqrt{6}}(r\bar{r} + g\bar{g} - 2b\bar{b})$.

We thus have an octet of color states plus a colorless singlet state. If this colorless singlet state existed, however, we would be able to observe it, not only via interactions with quarks, but as a free particle. Since do not observe this in nature, this restricts us to 8 gluons. The simplest group with a corresponding 8 generators is $SU(3)$. Under the assumption that $SU(3)$ is the local gauge symmetry of the strong interaction, we may proceed in a similar way as we did for QED. The gauge transformation is $\psi \to e^{ig_S\vec{\alpha}(x)\cdot\vec{T}}\psi$, where $\vec{T}$ is an eight component vector of the generators of $SU(3)$, often expressed via the Gell-Mann matrices, λ^a, as $t^a = \frac{1}{2}\lambda^a$, and the spinor ψ represents the fields corresponding to quarks.

This $SU(3)$ symmetry exactly expresses the color structure elucidated above – the Gell-Mann matrices are an equivalent presentation of the color combinations described above. Proceeding by analogy to QED, gauge invariance is achieved by introducing eight new degrees of freedom, G_μ^a, which are the gauge fields corresponding to the gluons, with the gauge covariant derivative then analogously taking the form $D_\mu \equiv \partial_\mu + ig_S G_\mu^a t^a$.

Recall from the QED derivation that the field strength tensor, $F^{\mu\nu}$ is a rank two

antisymmetric tensor which is manifestly gauge invariant and which describes the physical dynamics of the A_μ field. We would like to analogously define a term for the gluon fields. Repackaging this QED tensor, it is apparent that

$$[D_\mu, D_\nu] = D_\mu D_\nu - D_\nu D_\mu \tag{1.23}$$

$$= (\partial_\mu + iqA_\mu)(\partial_\nu + iqA_\nu) - (\partial_\nu + iqA_\nu)(\partial_\mu + iqA_\mu) \tag{1.24}$$

$$= \partial_\mu \partial_\nu + iq\partial_\mu A_\nu + iqA_\mu \partial_\nu + (iq)^2 A_\mu A_\nu - (\partial_\nu \partial_\mu + iq\partial_\nu A_\mu + iqA_\nu \partial_\mu + (iq)^2 A_\nu A_\mu) \tag{1.25}$$

$$= iq(\partial_\mu A_\nu - \partial_\nu A_\mu) + (iq)^2 (A_\mu A_\nu - A_\nu A_\mu) \tag{1.26}$$

$$= iq(\partial_\mu A_\nu - \partial_\nu A_\mu) + (iq)^2 [A_\mu, A_\nu]. \tag{1.27}$$

We proceed through this derivation to highlight that, in the specific case of QED, with its Abelian $U(1)$ gauge symmetry, the field commutator vanishes, leaving exactly the definition of $F_{\mu\nu}$ as described above, i.e.,

$$F_{\mu\nu} = \frac{1}{iq}[D_\mu, D_\nu]. \tag{1.28}$$

We may proceed to define an analagous field strength term for G_μ^a in a similar way:

$$G_{\mu\nu} = \frac{1}{ig_S}[D_\mu, D_\nu] \tag{1.29}$$

This has an extremely nice correspondence, but is complicated by the non-Abelian nature of $SU(3)$, with

$$G_{\mu\nu} = \partial_\mu (G_\nu^a t^a) - \partial_\nu (G_\mu^a t^a) + ig_s [G_\mu^a t^a, G_\nu^a t^a]. \tag{1.30}$$

in which the field commutator term is non-zero. In particular (since each term is summing over a, so we may relabel) as

$$[G_\mu^a t^a, G_\nu^b t^b] = [t^a, t^b] G_\mu^a G_\nu^b \tag{1.31}$$

and as $[t^a, t^b] = if^{abc}t^c$ for the Gell-Mann matrices, where f^{abc} are the structure constants of

$SU(3)$, we have

$$G_{\mu\nu} = \partial_\mu(G_\nu^a t^a) - \partial_\nu(G_\mu^a t^a) - g_s f^{abc} t^c G_\mu^a G_\nu^b \tag{1.32}$$

$$= t^a(\partial_\mu G_\nu^a - \partial_\nu G_\mu^a - f^{bca} G_\mu^b G_\nu^c) \tag{1.33}$$

$$= t^a G_{\mu\nu}^a \tag{1.34}$$

for $G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a - f^{abc} G_\mu^b G_\nu^c$.

This gives the component of the field strength corresponding to a particular gauge field a, where the first two terms have the familiar form of the QED field strength, while the last term is new, and explicitly related to the group structure via the f^{abc} constants. In terms of the physics content of the theory, this latter term gives rise to a gluon *self-interaction*, a distinguishing feature of QCD.

Similarly as in QED, a Lorentz invariant combination of field strength tensors may be made as $G_{\mu\nu} G^{\mu\nu}$. However, this is not manifestly gauge invariant. Under a gauge transformation U, the covariant derivative behaves as $D^\mu \to U D^\mu U^{-1}$, corresponding to $G^{\mu\nu} \to U G^{\mu\nu} U^{-1}$. The cyclic property of the trace thus ensures the gauge invariance of $\text{tr}(G_{\mu\nu} G^{\mu\nu})$, which we will write as $G_{\mu\nu}^a G_a^{\mu\nu}$ with the implied sum over generators a.

Packaging up the theory, it is tempting to copy the form of the QED Lagrangian, with the identifications we have made above:

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu}. \tag{1.35}$$

However this is not quite correct due to the $SU(3)$ nature of the theory. In terms of the physics, the Dirac fields ψ have associated color charge, which must interact appropriately with the G_μ fields. Mathematically, the generators t^a are 3×3 matrices, while the ψ are four component spinors. Adding a color index to the Dirac fields, i.e., ψ_i where i runs over the three color charges, and similarly indexing the generators t_{ij}^a, we may then express the $SU(3)$ gauge covariant derivative component-wise as

$$(D_\mu)_{ij} = \partial_\mu \delta_{ij} + i g_S G_\mu^a t_{ij}^a \tag{1.36}$$

where δ_{ij} is the Kronecker delta, as ∂_μ does not participate in the $SU(3)$ structure.

The Lagrangian then becomes

$$\mathcal{L} = \bar{\psi}_i(i(\gamma^\mu D_\mu)_{ij} - m\delta_{ij})\psi_j - \frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a. \tag{1.37}$$

and we have constructed QCD.

1.5 The Weak Interaction

One of the first theories of the weak interaction was from Enrico Fermi *TODO: cite*, in an effort to explain beta decay, a process in which an electron or positron is emitted from an atomic nucleus, resulting in the conversion of a neutron to a proton or proton to a neutron respectively. Fermi's hypothesis was of a direct interaction between four fermions. However, in the advent of QED, it is natural to wonder if a theory of based on mediator particles and gauge symmetries applies to the weak force as well. The modern formulation of such a theory is due to Sheldon Glashow, Steven Weinberg, and Abdus Salam *TODO: cite*, and is what we will describe in the following.

Considering emission of an electron, Fermi's theory involves an initial state neutron that transitions to a proton with the emission of an electron and a neutrino. Schematically *TODO: include figure*. This transition gives a hint that something slightly more complicated is happening than in QED: there is an apparent mixing between particle types.

Now, with the assumption there are mediators for such an interaction, we further know from beta decay and charge conservation that there must be at least two such degrees of freedom: e.g. one that decays to an electron and neutrino (W^-) and one that decays to a positron and neutrino (W^+). *TODO: Motivation for Z boson - grab Thomson 15.1.2.*

This leads to three degrees of freedom for the gauge symmetry of the weak interactions, so we thus need a theory which is locally invariant under transformations of a group with three generators. The simplest such choice is $SU(2)$. We may follow a very similar prescription as for QED and QCD: $SU(2)$ has three generators, which implies the existence of three gauge bosons, call them W^k_μ. The gauge transformation may be expressed as $\psi \to e^{ig_W \vec{\alpha}(x)\cdot\vec{T}}\psi$, where

in this case the generators are for $SU(2)$, which may be written in terms of the familiar Pauli matrices: $\vec{T} = \frac{1}{2}\vec{\sigma}$. The structure constants for $SU(2)$ are the antisymmetric Levi-Civita tensor, so the corresponding gauge covariant derivative is $D_\mu \equiv \partial_\mu + ig_W W_\mu^k t^k$, and the field strength tensor is $W_{\mu\nu}^k = \partial_\mu W_\nu^k - \partial_\nu W_\mu^k - \epsilon^{ijk} W_\mu^k W_\nu^k$.

The corresponding Lagrangian would thus be

$$\mathcal{L} = \bar{\psi}_i(i(\gamma^\mu D_\mu)_{ij} - m\delta_{ij})\psi_j - \frac{1}{4}W_{\mu\nu}^k W_k^{\mu\nu} \tag{1.38}$$

where indices i and j run over $SU(2)$ charges.

On considering some of the details, the universe unfortunately turns out to be a bit more complicated. However, this still provides a useful starting place for elucidating the theory of weak interactions. First off, let us consider the particle content, namely, what do the Dirac fields correspond to? This is still a theory of fermionic interactions with gauge bosons. However, we might notice that the fermion content of this theory is both a) broader than QCD, as we know experimentally (cf. beta decay) that both quarks and leptons (e.g. electrons) participate in the weak interaction and b) this fermion content seemingly has a large overlap with QED. In terms of the gauge bosons, we know that at both W^+ and W^- are electrically charged – this means that we expect some interaction of the weak theory with electromagnetism.

However, before diving deeper into this apparent connection between the weak interaction and QED, let us focus on the gauge symmetry. In QCD, the $SU(3)$ content of the theory is expressed via a contraction of color indices – the theory allows for transitions between quarks of one color and quarks of another. Thinking similarly in terms of $SU(2)$ transitions, the beta decay example is already fruitful – there is a transition between an electron and its corresponding neutrino, as well as between two types of quark. In particular, for the case of neutron (with quark content udd) and proton (with quark content udu), the weak interaction provides for a transtion from down to up quark.

Such $SU(2)$ dynamics are described via a quantity called *weak isospin*, denoted I_W with third component $I_W^{(3)}$, and can be thought of in a very similar way as color charge in QCD

(i.e. as the charge corresponding to the weak interaction). Since $SU(2)$ is 2×2, there are two such charge states for the fermions, denoted as $I_W^{(3)} = \pm\frac{1}{2}$. This means that the bosons must have $I_W = 1$ such that, by sign convention corresponding to electric charge, the W^+ boson has $I_W^{(3)} = +1$, the Z boson has $I_W^{(3)} = 0$, and the W^- boson has $I_W^{(3)} = -1$.

From conservation of electric charge, this means that transitions involving a $W^\pm$ are between particles that differ by ± 1 in both weak isospin $I_W^{(3)}$ and electric charge. We may thus line up all such doublets as:

$$\begin{pmatrix} \nu_e \\ e^- \end{pmatrix}, \begin{pmatrix} \nu_\mu \\ \mu^- \end{pmatrix}, \begin{pmatrix} \nu_\tau \\ \tau^- \end{pmatrix}, \begin{pmatrix} u \\ d' \end{pmatrix}, \begin{pmatrix} c \\ s' \end{pmatrix}, \begin{pmatrix} t \\ b' \end{pmatrix} \tag{1.39}$$

with the top corresponding to the lower weak isospin and electric charge particles, and the lower quark entries (d', etc) corresponding to the weak quark eigenstates (which are related to the mass eigenstates by the CKM matrix *TODO: more detail*). Similar doublets may be constructed for the corresponding anti-particles.

The fundamental structuring of these transitions around both electric and weak charge is again indicative of a natural connection. However, nature is again a bit more complicated than we have described. This is because the weak interaction is a *chiral* theory. For massless particles, chirality is the same as the perhaps more intuitive *helicity*. This describes the relationship between a particle's spin and momentum: if the spin vector points in the same direction as the momentum vector, helicity is positive (the particle is "right-handed"), and if the two point in opposite directions, the helicity is negative (the particle is "left-handed"). More concretely:

$$H = \frac{\vec{s} \cdot \vec{p}}{|\vec{s} \cdot \vec{p}|}. \tag{1.40}$$

For massive particles, this generalizes a bit – in the language of Dirac fermions that we have developed, we define projection operators

$$P_R = \frac{1}{2}(1 + \gamma^5) \quad \text{and} \quad P_L = \frac{1}{2}(1 - \gamma^5) \tag{1.41}$$

for right and left-handed chiralities respectively – acting on a Dirac field with such operators projects the field onto the corresponding chiral state.

Experimentally, this pops up via parity violation and the famous $V - A$ theory *TODO: more detail?*. For the scope of this thesis, it is sufficient to say that the weak interaction is only observed to take place for left-handed particles (and correspondingly, right-handed anti-particles). We therefore modify the theory stated above by projecting all fermions participating in the weak interaction onto respective chiral states – in particular, the $SU(2)$ gauge symmetry only acts on left-handed particles and right-handed anti-particles. We therefore modify the theory appropriately, denoting the chiral projected gauge symmetry as $SU(2)_L$, and similarly for the Dirac fields. In particular, the weak isospin doublets listed above must now be left-handed:

$$\begin{pmatrix} \nu_e \\ e^- \end{pmatrix}_L, \begin{pmatrix} \nu_\mu \\ \mu^- \end{pmatrix}_L, \begin{pmatrix} \nu_\tau \\ \tau^- \end{pmatrix}_L, \begin{pmatrix} u \\ d' \end{pmatrix}_L, \begin{pmatrix} c \\ s' \end{pmatrix}_L, \begin{pmatrix} t \\ b' \end{pmatrix}_L \tag{1.42}$$

and right-handed particle states are placed in singlets and assigned 0 charge under $SU(2)_L$ ($I_W = I_W^{(3)} = 0$).

With all of these assignments, let us revisit our guess at the form of the weak interaction Lagrangian. First, dwelling on the kinetic term $\bar{\psi}_i(i(\gamma^\mu D_\mu)_{ij}\psi_j$, we note that the assigning of left-handed fermions to isospin doublets and right-handed fermions to isospin singlets allows us to remove explicit $SU(2)$ indices by treating these as the fundamental objects, that is, for a single *generation* of fermions, we may write:

$$\bar{Q}i\gamma^\mu D_\mu Q + \bar{u}i\gamma^\mu D_\mu u + \bar{d}i\gamma^\mu D_\mu d + \bar{L}i\gamma^\mu D_\mu L + \bar{e}i\gamma^\mu D_\mu e \tag{1.43}$$

for left-handed doublets Q and L for quarks and electron fields respectively and right handed singlets u and d for up and down quark fields and e for electrons.

More concisely, and summing over the three generations of fermions, we may write

$$\sum_f \bar{f}i\gamma^\mu D_\mu f \tag{1.44}$$

where the f are understood to run over the fermion chiral doublets and singlets as above.

This then leaves our Lagrangian as

$$\mathcal{L} = \sum_f \bar{f} i \gamma^\mu D_\mu f - \frac{1}{4} W_{\mu\nu}^k W_k^{\mu\nu} \tag{1.45}$$

$$= \sum_f \bar{f} \gamma^\mu (i \partial_\mu - \frac{1}{2} g_W W_\mu^k \sigma_k) f - \frac{1}{4} W_{\mu\nu}^k W_k^{\mu\nu}, \tag{1.46}$$

where we have expanded the covariant derivative for clarity. You may note that we have dropped the mass term in the equation above – we will discuss this in detail in just a moment.

First, however, we return to our

Chapter 2

BEYOND THE STANDARD MODEL

The job of the experimental particle physicist is two-fold: observation and measurement of the various predictions of the Standard Model are important and exciting – the

Chapter 3

EXPERIMENTAL APPARATUS

Chapter 4

SIMULATION

Chapter 5

RECONSTRUCTION

Chapter 6

THE ANATOMY OF AN LHC SEARCH

In this thesis so far, we have set the theoretical foundation for the work carried out at the LHC. We have described how one may translate between this theoretical foundation and what we are actually able to observe with the ATLAS detector. We have further stepped through the process of simulating production of specific physics processes and their appearance in our detector, allowing us to describe how a hypothetical physics model would be seen in our experiment. The question then becomes: all of these pieces are on the table, what do we do with them? This chapter attempts to answer exactly that, setting up a roadmap for assembling these pieces into a statement about the universe.

6.1   Object Selection and Identification

As described in Chapter 5, there is a complicated set of steps for going from electrical signals in a detector to physics objects.

6.2   Defining a Signal Region

6.3   Background Estimation

6.4   Uncertainty Estimation

6.5   Hypothesis Testing

Chapter 7

SEARCH FOR PAIR PRODUCTION OF HIGGS BOSONS IN THE $b\bar{b}b\bar{b}$ FINAL STATE

This chapter presents two complementary searches for pair production of Higgs bosons in the final state. Such searches are separated based on the signal models being considered: resonant production, in which a new spin-0 or spin-2 particle is produced and decays to two Standard Model Higgs bosons, and non-resonant production, which is sensitive to the value of the Higgs self-coupling λ_{HHH}. Further information on the theory behind both channels can be found in Chapter *TODO: Fill in theory chapter.*

While the searches face many similar challenges and procede (in broad strokes) in a very similar manner, separate optimizations are performed to maximize the respective sensitivities for these two very different sets of signal hypotheses. More particularly, resonant signal hypotheses are (1) very peaked in values of the mass of the HH candidate system near the value of the resonance mass considered and (2) considered across a very broad range of signal mass hypotheses. The resonant searches are therefore split into resolved and boosted topologies based on Lorentz boost of the decay products, with the resolved channel as one of the primary focuses of this thesis. Further, several analysis design decisions are made to allow for sensitivity to a broad range of masses – in particular, though sensitivity is limited at lower values of m_{HH} relative to other channels *TODO: Combination, bbyy* due to the challenging background topology, retaining and properly reconstructing these low mass events allows the $b\bar{b}b\bar{b}$ channel to retain sensitivity up until the kinematic threshold at $250\,\mathrm{GeV}$.

In contrast, non-resonant signal hypotheses are quite broad in m_{HH}, and have a much more limited mass range, with Standard Model production peaking near $400\,\mathrm{GeV}$, and the majority of the analysis sensitivity able to be captured with a resolved topology. Even for

Beyond the Standard Model signal hypotheses, which may have more events at low m_{HH}, the non-resonant nature of the production allows the $b\bar{b}b\bar{b}$ channel to retain sensitivity while discarding much of the challenging low mass background. Such freedom allows for decisions which focus on improved background modeling for the middle to upper HH mass regime, resulting in improved modeling and smaller uncertainties than would be obtained with a more generic approach.

Both searches are presented in the following, with emphasis on particular motivations for, and consequences of, the various design decisions involved for each respective set of signal hypotheses.

7.1   Data and Monte Carlo Simulation

Both the resonant and non-resonant searches are performed on the full ATLAS Run 2 dataset, consisting of $\sqrt{s} = 13\,\text{TeV}$ proton-proton collision data taken from 2016 to 2018 inclusive. The

7.2   Triggers and Object Definitions

7.3   Analysis Selection

7.3.1   Resonant Search

7.3.2   Non-resonant Search

7.4   Background Estimation

fter the event selection described in Section **??** there are two major backgrounds, QCD and $t\bar{t}$, with relative proportions *TODO: Fill in appropriate ggF and VBF background composition*. Following the approach used for the resonant analysis, a fully data-driven estimate is used here. This is warranted due to the flexibility of the estimation method, as well as the high relative proportion of QCD background, and allows for the use of machine learning methods in the construction of the background estimate. However, it sacrifices an explicit treatment of the $t\bar{t}$ component. Performance of the background estimate on the $t\bar{t}$ component is thus

checked in Appendix *TODO: update ttbar studies/do for VBF*. The approach and its benefits over other methods are discussed below.

TODO: Do small background checks, text here kept from resonant Contributions of single Higgs processes to the background are checked in Appendix **??**. ZZ and HH backgrounds are checked in Appendix **??**. All are found to be negligible.

The foundation of the background estimate lies in the derivation of a reweighting function which matches the kinematics of events with exactly two b-tagged jets to those of events with four or more b-tagged jets. The reweighting function and overall normalization are derived in the control region. Systematic bias associated with extrapolating to the signal region in the Higgs candidate mass plane is assessed in the validation region. All derivation is done after the full event selection.

7.4.1   The Two Tag Region

Events in data with exactly two b-tagged jets are used for the data driven background estimate. The hypothesis here is that, due to the presence of multiple b-tagged jets, the kinematics of such events are similar to the kinematics of events in higher b-tagged regions (i.e. events with three and four b-tagged jets, respectively), and any differences can be corrected by a reweighting procedure. The region with three b-tagged jets is split into two b-tagging regions, with the $3b + 1$ loose region used as an additional signal region (see Section *TODO: Add ref*). The lower tagged $3b$ component ($3b + 1$ fail, as described in Section **??**) is reserved for validation of the background modelling procedure. Events with fewer than two b-tagged jets are not used for this analysis, as they are relatively more different from the higher tag regions.

The nominal event selection requires at least four jets in order to form Higgs candidates. For the four tag region, these are the four highest p_T b-tagged jets. For the three tag regions, these jets are the three b-tagged jets, plus the highest p_T jet satisfying a loosened b-tagging requirement. Similarly, and following the approach of the resonant analysis, the two tag region uses the two b-tagged jets and the two highest p_T non-tagged jets to form Higgs candidates.

Combinatoric bias from selection of different numbers of b-tagged jets is corrected as a part of the kinematic reweighting procedure through the reweighting of the total number of jets in the event. In this way, the full event selection may be run on two tagged events.

7.4.2 Kinematic Reweighting

The set of two tagged data events is the fundamental piece of the data driven background estimate. However, kinematic differences from the four tag region exist and must be corrected in order for this estimate to be useful. Binned approaches based on ratios of histograms (*TODO: Cite either 15+16 or full Run 2 VBF*) have been previously considered, but are limited in their handling of correlations between variables and by the "curse of dimensionality", i.e. the dataset becomes sparser and sparser in "reweighting space" as the number of dimensions in which to reweight increases, limiting the number of variables used for reweighting. This leads either to an unstable fit result (overfitting with finely grained bins) or a lower quality fit result (underfitting with coarse bins).

Note that even machine learning methods such as Boosted Decision Trees (BDTs), may suffer from this curse of dimensionality, as the depth of each decision tree used is limited by the available statistics after each set of corresponding selections (cf. binning in a more sophisticated way), limiting the expressivity of the learned reweighting function.

To solve these issues, a neural network based reweighting procedure is used here, following the success of the method used for the resonant search [**Abbott:2708605**]. This is a truly multivariate approach, allowing for proper treatment of variable correlations. It further overcomes the issues associated with binned approaches by learning the reweighting function directly, allowing for greater sensitivity to local differences and helping to avoid the curse of dimensionality.

Neural Network Reweighting

Let $p_{4b}(x)$ and $p_{2b}(x)$ be the probability density functions for four and two tag data respectively across some input variables x. The problem of learning the reweighting function between two

and four tag data is then the problem of learning a function $w(x)$ such that

$$p_{2b}(x) \cdot w(x) = p_{4b}(x) \tag{7.1}$$

from which it follows that

$$w(x) = \frac{p_{4b}(x)}{p_{2b}(x)}. \tag{7.2}$$

This falls into the domain of density ratio estimation, for which there are a variety of approaches. The method considered here is modified from [**NNloss**, **NNloss1**], and depends on a loss function of the form

$$\mathcal{L}(R(x)) = \mathbb{E}_{x \sim p_{2b}}[\sqrt{R(x)}] + \mathbb{E}_{x \sim p_{4b}}[\frac{1}{\sqrt{R(x)}}]. \tag{7.3}$$

where $R(x)$ is some estimator dependent on x and $\mathbb{E}_{x \sim p_{2b}}$ and $\mathbb{E}_{x \sim p_{4b}}$ are the expectation values with respect to the 2b and 4b probability densities. A neural network trained with such a loss function has the objective of finding the estimator, $R(x)$, that minimizes this loss. It is straightforward to show (Appendix **??**) that

$$\arg \min_R \mathcal{L}(R(x)) = \frac{p_{4b}(x)}{p_{2b}(x)} \tag{7.4}$$

which is exactly the form of the desired reweighting function.

In practice, to avoid imposing explicit positivity constraints, the substitution $Q(x) \equiv \log R(x)$ is made. The loss function then takes the equivalent form

$$\mathcal{L}(Q(x)) = \mathbb{E}_{x \sim p_{2b}}[\sqrt{e^{Q(x)}}] + \mathbb{E}_{x \sim p_{4b}}[\frac{1}{\sqrt{e^{Q(x)}}}], \tag{7.5}$$

with solution

$$\arg \min_Q \mathcal{L}(Q(x)) = \log \frac{p_{4b}(x)}{p_{2b}(x)}. \tag{7.6}$$

Taking the exponent then results in the desired reweighting function.

Variables and Results

The neural network is trained on a variety of variables sensitive to two vs. four tag differences. To help bring out these differences, the natural logarithm of some of the variables with a

large, local change is taken. The set of training variables for both ggF and VBF channels is shown in Table 7.1. *TODO: Update with final configuration/optimization when ready*

As mentioned, this number of jets variable is used to address the combinatoric bias of the two-tag region. The neural network used for the ggF reweighting has three densely connected hidden layers of 50 nodes each with ReLU activation functions and a single node linear output. The same applies to the neural network used for the VBF reweighting. These configuration demonstrates good performance in the modelling of a variety of relevant variables, including m_{HH}, when compared to a range of networks of similar size.

In practice, a given training of the reweighting neural network is subject to variation due to training statistics and initial conditions. An uncertainty is assigned to account for this (Section **??**), which relies on training an ensemble of reweighting networks [**DeepEnsembles**]. To increase the stability of the background estimate, the median of the predicted weight for each event is calculated across the ensemble. This median is then used as the nominal background estimate. This approach is indeed seen to be much more stable and to demonstrate a better overall performance than a single arbitrary training. Each ensemble used for this analysis consists of 100 neural networks, trained as described in Section **??**.

The training of the ensemble used for the nominal estimate is done in the kinematic Control Region. The prediction of these networks in the Signal Region is then used for the nominal background estimate. In addition, a separate ensemble of networks is trained in the Validation Region. The difference between the prediction of the nominal estimate and the estimate from the VR derived networks in the Signal Region is used to assign a systematic uncertainty associated with extrapolating in the Higgs Candidate mass plane. Further details on this systematic uncertainty are shown in Section **??**. Note that although the same procedure is used for both Control and Validation Region trained networks, only the median estimate from the VR derived reweighting is used for assessing the extrapolation uncertainty – no additional "uncertainty on the uncertainty" from VR ensemble variation is applied.

Each reweighted estimate is normalized such that the reweighted 2b yield matches the 4b

Table 7.1: Set of input variables used for tthe $2b$ to $4b$ reweighting in the ggF and VBF channels respectively.

ggF	VBF
1. $\log(p_T)$ of the 4th leading Higgs candidate jet	1. $\log(p_T)$ of the 4th leading Higgs candidate jet
2. $\log(p_T)$ of the 2nd leading Higgs candidate jet	2. $\log(p_T)$ of the 2nd leading Higgs candidate jet
3. $\log(\Delta R)$ between the closest two Higgs candidate jets	3. $\log(\Delta R)$ between the closest two Higgs candidate jets
4. $\log(\Delta R)$ between the other two Higgs candidate jets	4. $\log(\Delta R)$ between the other two Higgs candidate jets
5. Average absolute value of Higgs candidate jet η	5. Average absolute value of Higgs candidate jet η
6. $\log(p_T)$ of the di-Higgs system.	6. $\log(p_T)$ of the di-Higgs system.
7. ΔR between the two Higgs candidates	7. ΔR between the two Higgs candidates
8. $\Delta\phi$ between the jets in the leading Higgs candidate	8. $\Delta\phi$ between the jets in the leading Higgs candidate
9. $\Delta\phi$ between the jets in the subleading Higgs candidate	9. $\Delta\phi$ between the jets in the subleading Higgs candidate
10. $\log(X_{Wt})$, where X_{Wt} is the variable used for the top veto	10. $\log(X_{Wt})$, where X_{Wt} is the variable used for the top veto
11. Number of jets in the event	11. Number of jets in the event

yield in the corresponding training region. Note that this applies to each of the networks used in each ensemble, where the normalization factor is also subject to the procedure described in Section **??**. As the median over these normalized weights is not guaranteed to preserve this normalization, a further correction is applied such that the $2b$ yield, after the median weights are applied, matches the $4b$ yield in the corresponding training region. As no preprocessing is applied to correct for the class imbalance between $2b$ and $4b$ events entering the training, this ratio of number of $4b$ events ($n(4b)$) over number of $2b$ events ($n(2b)$) is folded into the learned weights. Correspondingly, the set of normalization factors described above is near 1 and the learned weights are centered around $n(4b)/n(2b)$ (roughly 0.01 over the full dataset). This normalization procedure applies for all instances of the reweighting (e.g. those used for validations in Section **??**), with appropriate substitutions of reweighting origin (here $2b$) and reweighting target (here $4b$).

Note that, though there are different trigger and pileup selections during each year, the statistically limited VBF channel benefits from combining all years together in performing the reweighting. The training input is the combined dataset from the years 2016 - 2018 with all configurations remaining unchanged except for the addition of the year of the given event as an input variable on top of the reweighting variables listed in Table 7.1. More detailed studies comparing the nominal split-year training and training on all years together for the VBF reweighting is presented in *TODO: ref appendix*. For the ggF channel, a similar approach was explored *TODO: ref appendix*, but was found to have minimal benefit over reweighting in each year separately. As the trigger selections for each year significantly impact the kinematics of each year, and thus categorizing by year is expected to reflect groupings of kinematically similar events and to provide a meaningful degree of freedom in the signal extraction fit, the split-year approach is kept by the ggF analysis.

7.5   Uncertainties

A variety of uncertainties are assigned to account for known biases in the underlying methods, calibrations, and objects used for this analysis. The largest such uncertainty is associated

with the kinematic bias inherent in deriving the background estimate away from the signal region. However, a statistical biasing of this same estimate has an effect of a similar magnitude. Additionally, due to the use of Monte Carlo for signal modelling and b-tagging calibration, uncertainties related to mismodellings in simulation must also be accounted for. These components, and their impact on this analysis, are described here in detail. Relative magnitudes of the uncertainties for each year are shown in Tables **??**, **??**, and **??** along with an estimate of the impact of the statistics of 4b data in the signal region on the total error. Note that, while the Poisson error (from 2b data statistics) is negligible relative to the bootstrap error in the bulk of the distribution, it becomes relevant in the high m_{HH} tail. The final statistical uncertainty used for the limit setting is therefore the sum (in quadrature) of these two components.

7.5.1 Statistical Uncertainties and Bootstrapping

There are two components to the statistical error for the neural network background estimate. The first is standard Poisson error, i.e., a given bin, i, in the background histogram has value $n_i = \sum_{j \in i} w_j$, where w_j is the weight for an event j which falls in bin i. Standard techniques then result in statistical error $\delta n_i = \sqrt{\sum_{j \in i} w_j^2}$, which reduces to the familiar $\sqrt{N}$ Poisson error when all w_j are equal to 1.

However, this procedure does not take into account the statistical uncertainty on the w_j due to the finite training dataset. Due to the large size difference between the two tag and four tag datasets, it is the statistical uncertainty due to the four tag training data that dominates that on the background. A standard method for estimating this uncertainty is the bootstrap resampling technique [**Bootstrap**]. Conceptually, a set of statistically equivalent sets is constructed by sampling with replacement from the original training set. The reweighting network is then trained on each of these separately, resulting in a set of statistically equivalent background estimates. Each of these sets is below referred to as a replica.

In practice, as the original training set is large, the resampling procedure is able to

be simplified through the relation $\lim_{n \to \infty} \text{Binomial}(n, 1/n) = \text{Poisson}(1)$, which dictates that sampling with replacement is approximately equivalent to applying a randomly distributed integer weight to each event, drawn from a Poisson distribution with a mean of 1.

Though the network configuration itself is the same for each bootstrap training, the network initialization is allowed to vary. It should therefore be noted that the bootstrap uncertainties implicitly capture the uncertainty due to this variation in addition to the previously mentioned training set variation.

The variation from this bootstrapping procedure is used to assign a bin-by-bin uncertainty which is treated as a statistical uncertainty in the fit. Due to practical constraints, a procedure for approximating the full bootstrap error band is developed which demonstrates good agreement with the full bootstrap uncertainty. This procedure is described below.

Calculating the Bootstrap Error Band

The standard procedure to calculate the bootstrap uncertainty would proceed as follows: first, each network trained on each bootstrap replica dataset would be used to produce a histogram in the variable of interest. This would result in a set of replica histograms (e.g. for 100 bootstrap replicas, 100 histograms would be created). The nominal estimate would then be the mean of bin values across these replica histograms, with errors set by the corresponding standard deviation.

In practice, such an approach is inflexible and demanding both in computation and in storage, in so far as we would like to produce histograms in many variables, with a variety of different cuts and binnings. This motivates a derivation based on event-level quantities. However, due to non-trivial correlations between replica weights, simple linear propagation of event weight variation is not correct.

We therefore adopt an approach which has been empirically found to produce results (for this analysis) in line with those produced by generating all of the histograms, as in the standard procedure. This approach is described below. Note that, for robustness to outliers and weight distribution asymmetry, the median and interquartile range (IQR) are used for

the central value and width respectively (as opposed to the mean and standard deviation).

The components involved in the calculation have been mentioned in Section **??** and are as follows:

1. Replica weight (w_i): weight predicted for a given event by a network trained on replica dataset i.

2. Replica norm (α_i): normalization factor for replica i. This normalizes the reweighting prediction of the network trained on replica dataset i to match the correponding target yield.

3. Median weight (w_{med}): median weight for a given event across replica datasets, used for the nominal estimate. Defined (for 100 bootstrap replicas) as

$$w_{med} \equiv \text{median}(\alpha_1 w_1, \ldots \alpha_{100} w_{100}) \tag{7.7}$$

4. Normalization correction (α_{med}): normalization factor to match the predicted yield of the median weights (w_{med}) to the target yield in the training region.

As mentioned in Section **??**, the *nominal estimate* is constructed from the set of median weights and the normalization correction, i.e. $\alpha_{med} \cdot w_{med}$.

For the bootstrap error band, a "varied" histogram is then generated by applying, for each event, a weight equal to the median weight (with no normalization correction) plus half the interquartile range of the replica weights: $w_{varied} = w_{med} + \frac{1}{2}\text{IQR}(w_1, \ldots, w_{100})$.

This varied histogram is scaled to match the yield of the nominal estimate. To account for variation of the nominal estimate yield, a normalization variation is calculated from the interquartile range of the replica norms: $\frac{1}{2}\text{IQR}(\alpha_1, \ldots, \alpha_{100})$. This variation, multiplied into the nominal estimate, is used to set a baseline for the varied histogram described above.

Denoting $H(\text{weights})$ as a histogram constructed from a given set of weights, $Y(\text{weights})$

as the predicted yield for a given set of weights, the final varied histogram is thus:

$$H(w_{med} + \frac{1}{2} \text{IQR}(w_1, \ldots, w_{100})) \cdot \frac{Y(\alpha_{med} w_{med})}{Y(w_{med} + \frac{1}{2} \text{IQR}(w_1, \ldots, w_{100}))} + \frac{1}{2} \text{IQR}(\alpha_1, \ldots, \alpha_{100}) \cdot H(\alpha_{med} w_{med})$$

(7.8)

where the first term roughly describes the behaviour of the bootstrap variation across the distribution of the variable of interest while the second term describes the normalization variation of the bootstrap replicas.

The difference between the varied histogram and the nominal histogram is then taken to be the bootstrap statistical uncertainty on the nominal histogram.

Figure *TODO: include figure* demonstrates how each of the components described above contribute to the uncertainty envelope for the 2017 Control Region and compares this approximate band to the variation of histograms from individual bootstrap estimates. The error band constructed from the above procedure is seen to provide a good description of the bootstrap variation.

7.5.2   Background Shape Uncertainties

To account for the systematic bias associated with deriving the reweighting function in the Control region and extrapolating to the Signal region, an alternative background model is derived in the Validation region. In contrast to previous work, this is done on the entire background model, due to the fully data-driven nature of the background used here. The alternative model and the baseline are consistent with the observed data in their regions and with each other. Differences between the alternative and baseline models are used to define a shape uncertainty on the m_{HH} spectrum, with a two-sided uncertainty defined by symmetrizing the difference about the baseline.

This uncertainty is split into two components to allow two independent variations of the m_{HH} spectrum: *TODO: HT vs quad splitting*

7.6   Statistical Analysis

7.7   Results