Exclusion limits on heavy neutral MSSM Higgs bosons $A/H$ decaying to a pair of top quarks in $pp$ collisions at $\sqrt{s} = 13$ TeV

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A search for heavy scalar $H$ and pseudoscalar $A$ neutral Higgs bosons at the LHC in their production in the gluon-fusion mechanism and their decays into a top quark pair is presented. This analysis uses the dataset with an integrated luminosity of 35.9 fb$^{-1}$ of $pp$ collision collected by the CMS experiment in 2016, at a center-of-mass energy of $\sqrt{s} = 13$ TeV. The results are interpreted in the context of the Minimal Supersymmetric Standard Model (MSSM). Interference effect between signal process and Standard Model $t\bar{t}$ production is being considered. Upper limits are set on the coupling modifier within the hMSSM benchmark scenario as a function of the Higgs mass $M_{A/H}$ and the ratio of vacuum expectation value of the Higgs doublet field $\tan \beta$ for $400 \leq M_{A/H} \leq 750$ GeV. Extrapolation of results is made for prediction of exclusion limits at luminosities of 100 and 1000 pb$^{-1}$.

INTRODUCTION

Despite the great triumph of the Standard Model (SM) upon the discovery of a scalar boson at a mass of 125 GeV by the ATLAS and CMS experiments in 2012 with subsequent measurements showing consistency with the SM Higgs boson, the SM is considered incomplete. The Higgs boson mass is known to suffer from quadratically divergent radiative corrections, Figure 1, at a cut-off scale $\Lambda$ beyond which the SM becomes invalid and new physics should appear. Supersymmetry (SUSY) is among the most appealing extensions to the SM which invokes a symmetry between bosons and fermions with the introduction of heavier superpartners to each particle and allowing for the cancellation of the radiative corrections.

In the low-energy SUSY scenario, the 2 Higgs Doublet Models (2HDMs) introduce two Higgs doublet fields $\Phi_1$ and $\Phi_2$ which are required to break the electroweak symmetry $[13]$. In the Type II 2HDMs, one of the fields couples to up type fermions and the other to down-type fermions. Within the Type II 2HDMs, the simplest extension to the Higgs sector, with the minimal gauge group and particle content $[10]$, is the Minimal Supersymmetric Standard Model. The spectrum of the MSSM Higgs sector consists of five Higgs states, two charged $H^\pm$, a neutral pseudoscalar $A$ and two neutral scalar $h$ and $H$, with the neutral Higgs states collectively denoted by $\phi = h, H, A$. At tree level, the phenomenology of the MSSM Higgs sector is fully determined by two free parameters, which is usually taken as the ratio of the vacuum expectation value (vev) of the Higgs doublet field, $\tan \beta = v_u/v_d$, and the pseudoscalar Higgs mass $M_A$.

The search for heavy neutral MSSM Higgs bosons focuses on two efficient decay channels, i.e. the decays of $A/H$ into $\tau^+\tau^-$ and $t\bar{t}$, which are complimentary in probing of the entire $[M_A, \tan \beta]$ parameter space $[9]$. With the strong coupling enhancement to the bottom quark associated production and the decay to taus due to the existence of a second Higgs doublet field, the high $\tan \beta$ region can be probed by searching for resonances decaying into taus. For low and moderate values of $\tan \beta$, the dominant production mode is the gluon fusion via a top loop with the heavy Higgs $A/H$ decaying predominately into a $t\bar{t}$ pair $[18]$. Figure 2, as the top-quark Yukawa coupling $\propto m_t/\tan \beta$ becomes large. In this analysis we based on the $H/A \rightarrow t\bar{t}$ decay process with particular focus on the $A \rightarrow t\bar{t}$ channel as $A \rightarrow WW/ZZ$ decays are forbidden by CP conservation making it the only way to discover such a particle.

Figure 2: Leading-order diagrams of gluon fusion (left) and $b$ quark associated production (middle and right) $[18]$.

Figure 3: Branching ratio of $H \rightarrow t\bar{t}$ (left) and $A \rightarrow t\bar{t}$ (right) in the $[M_A, \tan \beta]$ plane. $[9]$.
In this report, we investigate the production of heavy neutral Higgs bosons decaying into a top quark pair which opens up new regions in the \([M_A, \tan \beta]\) plane that have not been probed by previous searches\cite{7}. Despite unsuccessful attempts in finding signatures for new Higgs bosons in previous LHC runs, a large portion of the MSSM parameter space remains unexplored. With the current center-of-mass energy of 13 GeV pp collision and the data collected with the CMS detector at an integrated luminosity of 35.9 pb\(^{-1}\), expected limits may be set on the coupling strength to put constraints on the \([M_A, \tan \beta]\) parameter space of the MSSM. This analysis will focus on various procedures involved in the construction of the expected limits. The results are then extrapolated for estimating the sensitivity of the 14 TeV LHC run with luminosity up to 100 pb\(^{-1}\) and 1000 pb\(^{-1}\).

## THE hMSSM BENCHMARK SCENARIO

Radiative corrections produce considerable effects on the behavior beyond tree level in the MSSM, which is dependent on the choice of a large number of SUSY parameters. The hMSSM benchmark scenario \cite{9} refers to a particular choice of parametrization on the CP-conserving MSSM Higgs sector with the condition in the lightest Higgs boson mass, \(M_h = 125\) GeV. With proper assumptions given by the hMSSM scenario, the MSSM Higgs sector can again be characterized by only two inputs, i.e. \(M_A\) and \(\tan \beta\), as is like at the tree level.

In the hMSSM approach, all couplings of the Higgs particles to fermions and gauge bosons, involved in the evaluation of production cross-sections and decay widths of the Higgs particles, are dependent only on the values of \(\tan \beta\) and the mixing angle \(\alpha\) in the CP-even Higgs field, are summarized in Table I.

Table I: hMSSM Higgs couplings to fermions, \(u\) and \(d\), and gauge bosons, \(V\), normalized to the SM couplings.

<table>
<thead>
<tr>
<th>(H)</th>
<th>(g_{\Phi u u})</th>
<th>(g_{\Phi d d})</th>
<th>(g_{\Phi V V})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(h)</td>
<td>(\cos \alpha / \sin \beta)</td>
<td>(- \sin \alpha / \cos \beta)</td>
<td>(\sin (\beta - \alpha))</td>
</tr>
<tr>
<td>(H)</td>
<td>(\sin \alpha / \sin \beta)</td>
<td>(\cos \alpha / \cos \beta)</td>
<td>(\cos (\beta - \alpha))</td>
</tr>
<tr>
<td>(A)</td>
<td>(\cot \beta)</td>
<td>(\tan \beta)</td>
<td>0</td>
</tr>
</tbody>
</table>

By considering only the matrix element with the leading logarithmic terms for the radiative corrections\cite{22}, the hMSSM approach allows for simple expressions for the mass of the heavy scalar \(M_H\) and the mixing angle \(\alpha\):

\[
M_H^2 = \frac{(M_A^2 + M_Z^2 - M_h^2)(M_Z^2 \cos^2 \beta + M_h^2 \sin^2 \beta)}{M_Z^2 \cos^2 \beta + M_h^2 \sin^2 \beta - M_h^2} - \frac{M_A^2 M_Z^2 \cos 2\beta}{M_Z^2 \cos^2 \beta + M_h^2 \sin^2 \beta - M_h^2}\]

\(\alpha = - \arctan \left( \frac{(M_Z^2 + M_h^2) \cos \beta \sin \beta}{M_Z^2 \cos^2 \beta + M_h^2 \sin^2 \beta - M_h^2} \right)\)

**SIGNAL AND INTERFERENCE**

With the initial and final states of the Higgs production process being identical to the \(tt\) production, interference phenomenon would occur between the gluon-initiated loop production and the SM \(tt\) background production\cite{22}. The effect of interference is significant for (pseudo)scalar Higgs particles with masses above the \(tt\) production threshold, causing the signal shape to distort from a simple Breit-Wigner peak to a peak-dip structure\cite{11}, Figure 5.

The contribution of interference will result in a different normalization scheme for the signal samples and computation of the event yield since the negative contribution in the signal shape (the part below unity in Figure 5) still indicates a sign of deviation from the prediction\cite{22}. In the event generation of interference part of the signal shape in the \(m_{tt}\) spectrum, distributions with negative weights will also contribute to the final signal shape which puts a limitation on the sensitivity of the search for the signal resonance.

![Figure 4: Diagrams for gg → t\(\bar{t}\) production for (a) new physics and (b-d) Standard Model. Interference occurs between diagrams (a) and (c) and diagrams (a) and (b). Diagrams (a) and (d) do not interfere since they are both s-channel\cite{22}.](image)

![Figure 5: Illustration of the line shapes of the \(t\bar{t}\) mass spectrum of \(A \rightarrow t\bar{t}\) (left) and \(H \rightarrow t\bar{t}\) (right) with mass 750 GeV and total width \(\Gamma_H = 1\) GeV with contribution from pure signal (blue), interference (red) and overall combination (green)\cite{11}.](image)
EVENT GENERATION AND K FACTOR

To establish expected limits for estimating the sensitivity of the current experiment using the $A/H \to t\bar{t}$ decay channel, simulated data samples of signal and background events including interference contribution were produced using various event generators which are summarized in Table II. All events are generated at the center-of-mass energy of 13 TeV in pp collisions. The aspect of event reconstruction and selection is beyond the scope of this report and will not be discussed here.

The signal and interference data samples are generated for masses between 400 and 750 GeV and for decay widths between 1 and 50 %, relative to the mass. The data samples are refined to a binning of 50 GeV in mass and 0.5 % in width using mass and width morphing algorithms which is discussed in the next session. The production of scalar $H$ and pseudoscalar $A$ Higgs bosons via gluon fusion with top quarks final state is implemented in MadGraph5 [3] at LO only. To include higher order QCD corrections to the signal and interference cross-section, we apply a rescaling of the data samples by a $K$-factor, defined as the ratio of cross-section computed with the code SusHi 1.6.1 [10] at NNLO and that with the code MadGraph5 aMC@NLO 2.5.5 (MG) at LO, $K_{\text{NNLO}} = \sigma_{\text{NNLO}}/\sigma_{\text{LO}}$.

The $K$-factor is calculated for different masses corresponding to the simulated data samples. The dependence of the $K$-factor on decay width is evaluated in terms of the coupling which can be directly related to the width for a fixed mass. The SusHi code is configured using the MSTW2008 PDF set [1] following the choice from the LHC Higgs cross-section working group [5] and the MG code is configured using the NNPDF30 PDF set as recommended by the httbar working group (See [21]). The effect on the $K$-factor due to different pdf choice is measured to be within 5 %, with the NNPDF30 PDF set giving a slightly larger $K$-factor. As noted by [14], the choice of renormalization and factorization scales, $\mu_R$ and $\mu_F$, for perturbative QCD calculation of the cross-section [19] has a significant effect on the $K$-factor. In this analysis, a fixed scale of $\mu_F = \mu_R = m_{H/A}/2$ and a dynamical scale of $\mu_R = \mu_F = 1/2 \sum_i (m_i^2 + p_T^2(i))^{1/2}$, where $i$ runs over all final state particles and $m_i$ and $p_T(i)$ are their mass and transverse momentum respectively, are used following the recommended choice of [14]. To estimate the theoretical uncertainty on cross-section for various choice of $\mu_R$ and $\mu_F$, we vary the two scales in parallel up and down by a factor of two, Figure 7 (right).

However, in the computation of LO cross-sections for the process $gg \to A/H \to t\bar{t}$, which assumes stable top quarks final state, inconsistent results between SusHi and MG are obtained, Figure 7 (left). The deviation between the two results becomes significant at low Higgs masses and the reason for the deviation is still unclear.

The higher-order corrections for interference between the signal and background amplitudes have not yet been calculated [11] so its cross-section is only known to tree level. To evaluate the $K$-factor for interference contributions, we use the choice $K_I = \sqrt{K_F \times K_B}$, as suggested in Ref. [10], where $K_B = 1.77$ is the $K$-factor for the SM $t\bar{t}$ background. In this analysis, all $K$-factors are taken at a coupling of $g = 1$ and the $K$-factors for $ggH$ process is assumed to be identical to that of $ggA$ process. Figure 6 shows a summary of the $K$-factors obtained.

Table II: Summary of event generation for signal (top half) and background process (bottom half) used in the analysis [22].

<table>
<thead>
<tr>
<th>Process</th>
<th>$\sigma (\text{pb})$</th>
<th>$\mathcal{N}_{\text{norm}}$</th>
<th>order</th>
<th>generator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s_t$</td>
<td>0.53</td>
<td>2074732</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
<tr>
<td>$s_0$</td>
<td>0.30</td>
<td>1996866</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
<tr>
<td>$s_b$</td>
<td>0.19</td>
<td>2954567</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
<tr>
<td>$s_0$</td>
<td>0.13</td>
<td>1999935</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
<tr>
<td>$s_b$</td>
<td>0.09</td>
<td>1999935</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
<tr>
<td>$s_{\text{pseudoscalar}}$</td>
<td>1.17</td>
<td>2276394</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
<tr>
<td>$s_{\text{pseudo-scal}}$</td>
<td>0.68</td>
<td>1999940</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
<tr>
<td>$s_{\text{scalar}}$</td>
<td>0.44</td>
<td>1999949</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
<tr>
<td>$s_{\text{pseudoscalar}}$</td>
<td>0.31</td>
<td>1999932</td>
<td>LO</td>
<td>MGADAP5</td>
</tr>
</tbody>
</table>

Figure 6: $K$-factor for Higgs production via the $t\bar{t}$ decay channel for pseudoscalar $A$ (left) and scalar $H$ (right).

Figure 7: Ratio of cross-sections obtained from SusHi LO and MG LO results (left) and the uncertainty in cross-section on the normalization and factorization scales at LO, NLO and NNLO (right).
WIDTH AND MASS MORPHING

The simulation of signal and interference events is only performed for masses of \([400, 500, 600, 750]\) GeV and widths of \([2.5, 5, 10, 25, 50]\) % to save computing time. To obtain data samples with intermediate masses and widths for better prediction on the expected limits, various mass and width morphing algorithms are used. All morphing processes use information on the shapes of the simulated events from neighboring masses and widths and perform a rescaling of the event shapes, for both signal and interference contribution. For the mass morphing algorithm, a scaling based on NonLinearPostFractions, which is implemented in RooMomentMorph \([2]\), is used. Such scaling is found to best describe the dependence of the cross-section on the Higgs boson mass. Whereas for the width morphing algorithm, a hyperbolic and linear interpolation is used for signal and interference process respectively.

It should be noted that all data samples are generated according to the background only (SM) hypothesis which corresponds to a coupling of \(g/g_{\text{SM}}\) \(\approx 1\). In the (h)MSSM, the LO (differential) cross-section for the process \(ggA \to t\bar{t}\) (which is asymptotically equal to the \(ggA\) production cross-section as the branching ratio is close to unity in the low tan \(\beta\) and high \(M_{H/A}\) regime) for the signal contribution is given by \([11]\)

\[
\frac{d\sigma_S}{dz} = \frac{3\alpha_s G_F^2 m_t^2}{8192 \pi s^2} \sum_{q} |\tilde{\beta}_{\text{Q}}^q g_{bqtt} \sum_{f} g_{bqq} A_f^p (\bar{\xi}_f)|^2 (s - M_{\Phi}^2)^2 + \frac{1}{4\sqrt{2\pi}} M_{\Phi} \beta_\Phi
\]

which implies \(\sigma_S \propto g_{bqtt}^2\). The decay widths for the process \(A/H \to t\bar{t}\) is given by \([11]\)

\[
\Gamma(\Phi \to t\bar{t}) = N_c G_F m_t^2 \frac{g_{bqtt}^2 M_{\Phi} \beta_\Phi}{4\sqrt{2\pi}}
\]

which implies \(\Gamma \propto g_{bqtt}^2\) (total width \(\sim\) partial width for low tan \(\beta\)). Therefore, the cross-section for signal events, generated using the MG LO generator, must first be rescaled to a unit coupling along the hMSSM prediction and then to the desired width (which is proportional to \(g_{bqtt}^2\)). As shown in Figure 8, the scaling will be equivalent to moving along the hMSSM line (blue) down to a unit coupling and then move up or down to the desired width. Therefore, when moving along a fixed width, the signal cross-section will scale as \(\sigma_{\text{hMSSM}}^\text{data} \propto g_{bqtt}^2\). In many cases, the interference amplitude is given by the square root of the amplitudes for the processes that interfere, hence the interference cross-section will scale as \(\sigma_{\text{hMSSM}}^\text{data} \propto g_{bqtt}^2\). The dependence can be observed from the MG result, Figure 9. This implies:

\[
\frac{\sigma_S^\text{data}}{g_{bqtt}^2} \propto \frac{\sigma_{\text{hMSSM}}^\text{data}}{g_{bqtt}^2} \propto \frac{1}{g^2} \propto \frac{1}{\Gamma}
\]

which justifies the use of hyperbolic interpolation for signal process. The dependence is checked with the MG result as shown in Figure 10 (left). For the interference process, the cross-section does not follow any simple relation so a linear interpolation is used by default, see Figure 10 (right).

Figure 8: Dependence between coupling\(^2\) \((1/ \tan \beta^2)\) and decay width. The blue and black lines indicate the results for total and partial widths (to \(t\bar{t}\)) respectively. The shaded region corresponds to non-physical results with a branching ratio larger than 100%.

Figure 9: MG results for dependence of cross-section on coupling for sign (left) and interference (right) process at \(M_A = 400\) GeV and width = 40 GeV.

Figure 10: MG results for hyperbolic and linear fitting of \(ggA\) cross-section with respect to width for signal (left) and interference (right) process respectively.

To obtain exclusion limits for all available mass points, data samples with widths below 2.5% are needed. Instead of generating new MC samples, we introduce an extrapolation scheme for producing signal and interference shapes at 1% width. The extrapolation is based on the assumption that signal and interference samples for
widths at a small enough interval share the same shape in their \( t\bar{t} \) invariant mass spectrum. By comparing the normalized signal and interference shapes between the available 2.5% and 5% widths, Figure 11, we can see that the shapes at the two different widths share similar features and the ratio of the number of events for each bin at 2.5% width to 5% width are reasonably close to one within statistical fluctuation.

![Figure 11: Comparison of the normalized signal (left) and interference (right) shapes for \( ggA \) process between a width of 2.5 and 5% at \( M_A = 400 \) (left) and 600 (right) GeV.](image1)

To obtain the shapes at 1% width, the ratio of cross-section of 2.5% width to 1% width is calculated using LO MG for all available masses. Since the width is a free parameter in MG, we need to fix the corresponding coupling to the hMSSM value using SusHi. This is achieved by scanning across a range of couplings with small enough intervals until the desired width is crossed. The final value of the input coupling is obtained by linear interpolation between the two coupling values to the desired width. The final cross-section is obtained by rescaling the it by a factor of \( g^4 \) for the signal process or by a factor of \( g^2 \) for the interference process.

A summary of the cross-section ratio can be found in Figure 12. The large deviation for interference process at masses between 600 and 700 GeV is due to the transition from a negative cross-section (negative interference) to a positive cross-section, resulting in large statistical fluctuations. The ratio for the scalar \( H \) is assumed to be the same as the pseudoscalar \( A \) for convenience and the ratio for interference process is assumed to be 1 for all mass values regardless of the Higgs boson type. The ratio is crosschecked with the ratio of the number of events of 2.5% width to 5% width available from the data samples, see Figure 13.

![Figure 12: Cross section ratio between widths of 1 and 2.5% (solid line) and between widths of 2.5 and 5% (dashed line) for \( ggA \) (blue) and \( ggH \) (green) process.](image2)

The ratio obtained from the data samples is the statistical average for all related processes for the bin with the maximum event count. There is a good agreement between the ratios obtained from MG and that from the data samples for the signal process within statistical fluctuation. However, for the interference process, a considerable deviation is observed. Since the calculation of cross-section from MG only consider stable top quarks final state, the effect from decays into 1-jets may introduce considerable corrections to the final cross-section that is not accounted for in the MG calculation.

![Figure 13: Comparison of cross-section ratio between widths of 2.5 and 5% obtained from MG (blue solid line) and from actual data samples (dashed lines) for signal (left) and interference (right) \( ggA \) process.](image3)

**EVALUATION OF EXPECTED LIMITS**

The exclusion limits on the MSSM parameter space are derived from a frequentist significance test, known as the asymptotic CLs method\(^8\), using a profile likelihood ratio as a test statistic. We express our results as a limit on the coupling modifier, \( \kappa = g/g_{\text{SM}}^{t\bar{t}} \), defined as the ratio of best-fit coupling to the expected SM Higgs coupling (in the same sense as \( g_{A/Ht}^{t\bar{t}} \) in Table I). The sensitivity of an experiment is characterized by the median significance, using pseudo-data generated from the \( \kappa = 1 \) (background only) hypothesis, with which one rejects values of \( \kappa \) incompatible with the MSSM prediction at 95% confidence level (CL).

Suppose the expected yield for the signal process is \( s_i \), which may be scaled by a signal strength factor \( \mu \), and that for the background is \( b_i \) in each bin \( i \) of the reconstructed \( n_{t\bar{t}}\cos\theta_{t\bar{t}lep} \) mass distribution, where \( \theta_{t\bar{t}lep} \) is the angle between \( \vec{p}_{t\bar{t}} \) in the \( t\bar{t} \) rest frame and \( \vec{p}_{t\bar{t}} \) in the lab frame\(^2\). The number of observed events \( n_i \) in the \( i \)-th bin follows the Poisson distribution

\[
Pois(n_i | \mu \cdot s_i + b_i) = \frac{(\mu \cdot s_i + b_i)^{n_i}}{n_i!} e^{-(\mu \cdot s_i + b_i)}
\]  

(7)
The systematic uncertainties for the predicted signal and background yields are modeled by nuisance parameters $\theta$ (see also Ref[17]) so that the likelihood function takes the form

$$L_{\text{data}}(\mu, \theta) = \prod_{i=1}^{N} \text{Pois}(n_i; \mu \cdot s_i(\theta) + b_i(\theta))p(\theta)$$

where $p(\theta)$ is a probability density function for all nuisance parameter measurements.

To set exclusion limits on a signal hypothesis, we define a profile likelihood ratio as a test statistic

$$q_\mu = -2 \ln \left( \frac{L_{\text{data}}(\mu \cdot s(\hat{\theta}_\mu) + b(\hat{\theta}_\mu))}{L_{\text{data}}(\mu \cdot s(\hat{\theta}_\mu) + b(\theta))} \right), \quad 0 \leq \hat{\mu} < \mu,$$

Here $\theta_\mu$ denotes the value of $\theta$ that maximizes the likelihood in the numerator under the hypothesis of a signal of strength $\mu$, and the denominator is the globally maximized likelihood under the constraint $0 \leq \hat{\mu} < \mu$. The last constraint is required for one-sided limits on the Higgs boson production rate. A higher values of $q_\mu$ represents greater incompatibility between the observed data and the hypothesized $\mu$. The CLs limit is constructed based on the tail probabilities for which one would obtain a value for the test statistic $q_\mu$ larger than the observed value $q_\mu^{\text{obs}}$ for the signal + background and for the background-only hypothesis (See also[6]):

$$\text{CL}_{s+b} = P(q_\mu \geq q_\mu^{\text{obs}} | \mu \cdot s + b),$$

$$\text{CL}_b = P(q_\mu \geq q_\mu^{\text{obs}} | b),$$

from which we obtain the exclusion at 95% CL ($\alpha = 5\%$) by adjusting the value of $\mu$ until we reach the condition

$$\text{CL}_\alpha = \frac{\text{CL}_{s+b}}{\text{CL}_b} \leq \alpha.$$ (12)

In the asymptotic CLs method, approximate formulae for high statistics are obtained. From Wald approximation, the test statistic can be written as

$$q_\mu = \begin{cases} \left(\frac{\hat{\mu} - \bar{\mu}}{\sigma}\right)^2 & \hat{\mu} < \mu, \\ 0 & \hat{\mu} > \mu, \end{cases}$$

where $\hat{\mu}$ is assumed to follow a Gaussian distribution with a standard deviation $\sigma$. For a blinded analysis, the observed data is replaced by a representative dataset, called the Asimov dataset, containing both contribution from background processes and a SM Higgs boson with $m_h = 125$ GeV. Multiple upper limits at 95 % CL are obtained as the MC generated pseudo-data will contain statistical fluctuations. Expected limits are therefore quoted in terms of a median expectation with associated ±1 and ±2 $\sigma$ bands [8]. The values of $\mu$ are then expressed in terms of the coupling modifier $\kappa$ for making exclusion.

**EXCLUSION IN MSSM PARAMETER SPACE**

Expected exclusion regions in the MSSM $[M_A, \tan \beta]$ parameter space is obtained by comparing the hMSSM prediction with the median expectation limit on the coupling modifier computed from the MC simulated data templates using the asymptotic CLs method. A crossing between the hMSSM prediction and the expected limits indicates the value of coupling above which can be excluded. Those values correspond to a prediction on the number of event that is incompatible with the expected value from the background only hypothesis in 95 % of the time. The coupling is then related to the value of $\tan \beta$ by the relation shown in Table 1 i.e. $g_{A/H} = \cot \beta$ and $g_{H/H} = \sin \alpha / \sin \beta$. The value of the mixing angle $\alpha$ is fixed by the values of $M_A$ and $\tan \beta$ from Eq[2].

![Figure 14: Expected limits on the coupling modifier for pseudoscalar $A$ with $M_A = 400$ GeV (left) and for scalar $H$ with $M_H = 750$ GeV (right) compared with the hMSSM predicted value (blue line). Regions shaded in red are limits obtained from extrapolated data samples. Regions shaded in blue are limits obtained from linear extrapolation of expected limits at 1 and 1.5 %.](image)

Examples of expected limits with hMSSM prediction is shown in Figure 14 for pseudoscalar $A$ with $M_A = 400$ GeV and for scalar $H$ with $M_H = 750$ GeV. In general, the analysis on the pseudoscalar $A$ via the $t\bar{t}$ decay channel will have a higher sensitivity than the scalar $H$ as the decays to vector bosons are forbidden for $A$ due to CP conservation. The sensitivity is also reduced at higher Higgs boson mass because of the smaller cross-section limited by the current pp collision energy. Extremely small values of $\tan \beta \lesssim 0.3$ (or equivalently large values of coupling) are generally forbidden by theory due to the constrain on the Yukawa coupling of the heavy top quark[10]. Therefore, if the expected limit is not crossed by the hMSSM prediction for sufficiently a large coupling, i.e. for $\tan \beta \lesssim 0.3$, then we will assume no exclusion is made for a Higgs boson at that particular mass. In Figure 14 we can see that the theory prediction (blue line) is well below the medium expected limit for a scalar $H$ with $M_H = 750$ GeV even for a relatively high coupling, therefore no exclusion at $M_H = 750$ is made.

The broadening of the limit band at higher widths as
shown in Figure 14 is one of the observations that has not been fully explained yet. The effect is most prominent at higher Higgs masses for both scalar $H$ and pseudoscalar $A$. In general, the limit band will widen when the effects from systematic uncertainties take over or when the statistical uncertainties become significant due to low event counts. For these to have dependence on width, we investigate the combined signal shapes at different widths for various masses of the Higgs bosons which include all contributions from signal and positive and negative interference. The result is shown in Figure 15 and Figure 16 for pseudoscalar $A$ and scalar $H$ respectively. A significant cancellation between signal and interference events at higher widths is observed for a mass of $M_{A/H} = 750$ GeV but not for $M_{A/H} = 400$ GeV. The resultant low signal count at higher widths for a high mass Higgs boson may have caused the observed widening of limit bands. Further validation is required to find out the effect of signal event cancellation on the resultant expected limits.

Figure 15: Combined signal shapes for a pseudoscalar $A$ of $M_A = 400$ GeV (top) and $M_A = 750$ GeV (bottom) at 2.5% (left), 25% (middle) and 50% (right) widths.

Figure 16: Combined signal shapes for a scalar $H$ of $M_H = 400$ GeV (top) and $M_H = 750$ GeV (bottom) at 2.5% (left), 25% (middle) and 50% (right) widths.

**SYSTEMATIC UNCERTAINTIES**

The systematic uncertainties are treated as nuisance parameters in the statistical procedure for finding the expected limits on the model parameters. This analysis includes approximately 797 nuisance parameters modeled with simple Gaussian constraints. Most of these uncertainties involved are statistical in nature, i.e. due to the finite size of the simulated samples used to model the expected signal and background yields. Nuisance parameters of this kind are collectively called bin-by-bin uncertainties which can take different values in each bin.

There are also other uncertainties which can be theoretical or experimental in nature. The main theoretical uncertainties affecting the signal yield include the QCD scale uncertainty, i.e. uncertainties on the renormalization and factorization scales due to missing higher order QCD corrections, and uncertainties in Parton Distribution Functions (PDFs). Experimental uncertainties in integrated luminosity, pile-up and trigger efficiency also play a major role in affecting the normalization and shape of the reconstructed $m_{t\bar{t}}$ distribution.

In this analysis, we would like to estimate for the expected limits in three different luminosity scenarios: 35.9 pb$^{-1}$ (nominal), 100 pb$^{-1}$ and 1000 pb$^{-1}$. Upon extrapolation to higher luminosities, the effect of statistical uncertainties on the expected limits will become significant as the number of simulated data samples does not go up with the increased luminosity. To measure the effect of a nuisance parameter $\theta$ on a parameter of interest $r$ (the signal strength), we define the impact as the shift $\Delta r$ that is induced when $\theta$ is fixed and moved to its $+1\sigma$ or $-1\sigma$ value, with all other nuisance parameters profiled as normal. Figure 17 shows the impacts of nuisance parameters with data samples extrapolated to 1000 pb$^{-1}$ luminosity. Only 30 nuisance parameters with largest impacts are shown. The impacts are evaluated for a pseudoscalar $A$ with $M_A = 750$ GeV at 10% width.

![Figure 17: Impacts of nuisance parameters on the signal strength $r$ with data extrapolated at 1000 pb$^{-1}$ luminosity. Only 30 nuisance parameters with largest impacts are shown. The impacts are evaluated for a pseudoscalar $A$ with $M_A = 750$ GeV at 10% width.](image)
the largest impacts.

To reduce the effect of statistical uncertainties without recourse to simulating more data samples, we may apply a scaling of the constraints on the bin-by-bin uncertainties according to the ratio of luminosity between the extrapolated data and the nominal data (lumiscale). This is equivalent to scaling the width of the Gaussian constraint on each nuisance parameter, that corresponds to a bin-by-bin uncertainty, by a factor of $1/\sqrt{\text{lumiscale}}$ [12]. Such scaling is based on the assumption that the error on the fitted value of the nuisance parameter should be proportional to $1/\sqrt{N}$ for a large enough number of simulated data samples $N$.

**RESULTS**

The 95% CL upper limits on $\tan \beta$ as a function of the pseudoscalar Higgs boson mass $M_A$ or the scalar Higgs boson mass $M_H$ are set for the hMSSM benchmark scenario using data considering only the pseudoscalar $A$ and data considering only the scalar $H$ respectively for mass values of $400 \leq M_{A/H} \leq 750$ GeV with 50 GeV binning. In this analysis, upper limits for data at different luminosities are considered, i.e. at $L = 35.9$ pb$^{-1}$ (nominal), 100 pb$^{-1}$ and 1000 pb$^{-1}$. The extrapolated results at higher luminosities are obtained by scaling all signal and background shapes from the nominal data samples by the luminosity factor, i.e. lumiscale $= 2.79$ for $L = 100$ pb$^{-1}$ and lumiscale $= 27.86$ for $L = 1000$ pb$^{-1}$. In Figure 18, the expected exclusion regions for the MSSM are shown for the pseudoscalar $A$ and the scalar $H$ at the three different luminosities discussed above. The excluded values of $\tan \beta$ for the different mass hypotheses are listed in Table III and Table IV for the pseudoscalar $A$ and scalar $H$ respectively. The results allow us to estimate the sensitivity in the search for heavy neutral MSSM Higgs bosons via the $t\bar{t}$ decay channel with the luminosities and center-of-mass energy reached by the LHC.

To study the effect of bin-by-bin uncertainties on the expected exclusion limits, the statistical procedure is repeated with all the nuisance parameters corresponding to the bin-by-bin uncertainties removed. The expected limits at 95% CL on the coupling modifier, obtained with and without bin-by-bin uncertainties at three different luminosities, as a function of the width at two different mass values $M_{A/H} = 400$ GeV and $M_{A/H} = 750$ GeV for both pseudoscalar $A$ and scalar $H$ are shown in Figure 19. The excluded values of $\tan \beta$ for the different mass hypotheses, obtained without considering bin-by-bin uncertainties, are listed in Table V and Table VI for the pseudoscalar $A$ and scalar $H$ respectively.

As expected, the $t\bar{t}$ decay channel is most sensitive to the low $\tan \beta$ regime where the branching ratio of $H/A \to t\bar{t}$ is close to 1. The sensitivity goes down with the decrease in cross section at higher mass values due to limitation from the pp collision energy. The sensitivity for the scalar $H$ is considerably lower than the pseudoscalar $A$ due to the extra decays into vectors bosons $H \to VV$ which are forbidden for the pseudoscalar due to CP conservation.

Figure 18: The 95% CL expected exclusion regions considering only a pseudoscalar $A$ (left) or only a scalar $H$ (right) at nominal 35.9 pb$^{-1}$ (top), 100 pb$^{-1}$ (middle) and 1000 pb$^{-1}$ (bottom) luminosities. All results include bin-by-bin uncertainties. The areas below the red solid lines are expected to be excluded.

<table>
<thead>
<tr>
<th>$M_A$ [GeV]</th>
<th>$L$ [pb$^{-1}$]</th>
<th>$\tan \beta$:</th>
<th>exp.</th>
<th>exp.</th>
<th>exp.</th>
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</tr>
<tr>
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<td></td>
<td>$&lt; 1.68$</td>
<td>$&lt; 1.89$</td>
<td>$&lt; 2.06$</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td></td>
<td>$&lt; 1.44$</td>
<td>$&lt; 1.62$</td>
<td>$&lt; 1.78$</td>
<td></td>
</tr>
<tr>
<td>550</td>
<td></td>
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<td></td>
<td>$&lt; 0.96$</td>
<td>$&lt; 1.08$</td>
<td>$&lt; 1.22$</td>
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</tr>
<tr>
<td>650</td>
<td></td>
<td>$&lt; 0.78$</td>
<td>$&lt; 0.90$</td>
<td>$&lt; 1.02$</td>
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<tr>
<td>700</td>
<td></td>
<td>$&lt; 0.66$</td>
<td>$&lt; 0.75$</td>
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<tr>
<td>750</td>
<td></td>
<td>$&lt; 0.52$</td>
<td>$&lt; 0.63$</td>
<td>$&lt; 0.72$</td>
<td></td>
</tr>
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</table>

Table III: The 95% CL expected exclusion limits on $\tan \beta$ for MSSM considering only a pseudoscalar $A$ with bin-by-bin uncertainties.
At some particular values of the coupling. However, of cancellation between signal and interference contribu-
tions at higher widths. The bump is speculated to be a result
of $\tan \beta$, but is much more prominent for $H$

A bar (–) indicates that no value of $\tan \beta \geq 0.3$ is excluded

Table IV: The 95% CL expected exclusion limits on $\tan \beta$
for MSSM considering only a pseudoscalar $H$ with bin-
by-bin uncertainties.

As seen from Figure 19, the effect from bin-by-bin un-
certainties is more prominent at higher luminosities as the
gap between the lines of the expected limits with and
without bin-by-bin uncertainties are getting larger. One
interesting feature to note from Figure 19 is the bump at
a higher mass value for both pseudoscalar $A$ and scalar
$H$ but is much more prominent for $A$. The size of the
bump seems to increase with mass with the peak shifting
to higher widths. The bump is speculated to be a result
of cancellation between signal and interference contribu-
tions at some particular values of the coupling. However,
no conclusion is made at the current stage yet.

Table V: The 95% CL expected exclusion limits on $\tan \beta$
for MSSM considering only a pseudoscalar $A$ without bin-
by-bin uncertainties.

<table>
<thead>
<tr>
<th>$M_H$ [GeV]</th>
<th>$L$ [pb$^{-1}$]</th>
<th>35.9</th>
<th>100</th>
<th>1000</th>
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<td>550</td>
<td>&lt; 0.87</td>
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<td>&lt; 1.15</td>
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<td>&lt; 0.62</td>
<td>&lt; 0.73</td>
<td>&lt; 0.84</td>
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</tr>
<tr>
<td>700</td>
<td>–</td>
<td>&lt; 0.58</td>
<td>&lt; 0.68</td>
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</tr>
<tr>
<td>750</td>
<td>–</td>
<td>&lt; 0.45</td>
<td>&lt; 0.60</td>
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Table VI: The 95% CL expected exclusion limits on $\tan \beta$
for MSSM considering only a pseudoscalar $H$ without jggj
bin-by-bin uncertainties. A bar (–) indicates that no value
of $\tan \beta \geq 0.3$ is excluded

The results from the pseudoscalar $A$ and the scalar $H$
are combined to improve the sensitivity of the search. In
principle, this is achieved by simultaneously fitting the
data with the processes $gg \rightarrow A/H \rightarrow t\bar{t}$. For simplicity,
we only extend the exclusion limits in $M_H$ to the corre-
spnding limits in $M_A$ using the relation from Eq. 1. For
small values of $\tan \beta$, $M_A$ is generally smaller than $M_H$,
as shown in Figure 20, but becomes degenerate at high
masses. Therefore, at the current sensitivity of $H$, only
exclusion limits at $M_H = 400$ GeV can be extended which
correspond to a mass of $M_A \sim 350$ GeV. The combined
result is shown in Figure 21.

Table VI: The 95% CL expected exclusion limits on $\tan \beta$
for MSSM considering only a pseudoscalar $A$ without bin-
by-bin uncertainties.

<table>
<thead>
<tr>
<th>$M_H$ [GeV]</th>
<th>$L$ [pb$^{-1}$]</th>
<th>35.9</th>
<th>100</th>
<th>1000</th>
</tr>
</thead>
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<td>&lt; 1.20</td>
<td>&lt; 1.36</td>
<td>&lt; 1.51</td>
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<td>&lt; 1.37</td>
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<tr>
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<td>&lt; 1.27</td>
<td>&lt; 1.50</td>
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<tr>
<td>550</td>
<td>&lt; 0.91</td>
<td>&lt; 1.10</td>
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<td>600</td>
<td>&lt; 0.80</td>
<td>&lt; 0.97</td>
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<tr>
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<td>&lt; 0.80</td>
<td>&lt; 0.99</td>
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</tr>
<tr>
<td>700</td>
<td>&lt; 0.46</td>
<td>&lt; 0.65</td>
<td>&lt; 0.80</td>
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<tr>
<td>750</td>
<td>–</td>
<td>&lt; 0.56</td>
<td>&lt; 0.72</td>
<td></td>
</tr>
</tbody>
</table>

Figure 19: Expected limits on coupling modifier obtained
at nominal 35.9 pb$^{-1}$ (red), 100 pb$^{-1}$ (green) and 1000 pb$^{-1}$
(blue) luminosities with (square) and without (cross)
bin-by-bin uncertainties in comparison to the hMSSM
predicted value (black) for 400 GeV (left) and 750 GeV
(right) mass for pseudoscalar $A$ (top) and scalar $H$ (bottom).

Figure 20: Relation between pseudoscalar mass $M_A$ and
scalar mass $M_H$ (left) and relation between pseudoscalar mass $M_A$ and the mixing angle $\alpha$ (right).
All values are calculated at tree level.
Finally, the implementation of the nuisance parameter constraints scaling is not matured yet. The method is tested with a scaling that corresponds to a luminosity of 1000 pb$^{-1}$. Nonsensical results with expected limits on the coupling modifier smaller than that in the case without bin-by-bin uncertainties are obtained, Figure 22. The crossing of the medium expected limits with the lower blue tail of the hMSSM prediction will mean an exclusion of high $\tan \beta$ regions which is not reachable by the $t\bar{t}$ decay channel.

A check on the impacts of nuisance parameters is performed for a pseudoscalar $A$ with $M_A = 750$ GeV at 10% width. There is a significant reduction in the impacts compared with the result without a constraint scaling. However, the impacts are tilted towards a positive effect on the signal strength $r$. There also arises the problem that after the fit some nuisance parameters are at their boundary value. Further checks on the convergence of limits with the likelihood scan may be performed but are left for future investigation.

In conclusion, the sensitivity of the search for heavy pseudoscalar $A$ and scalar $H$ Higgs boson decaying into a top quark pair with 35.9 pb$^{-1}$ pp collision data and center-of-mass energy at 13 TeV recorded by the CMS experiment has been estimated with simulated data samples. The analysis takes into account the interference effects between the signal process and the SM $t\bar{t}$ background. The results are interpreted in the context of the MSSM with the hMSSM benchmark scenario. Exclusion limits are set in the $[M_A, \tan \beta]$ parameter space for $400 \leq M_A/\tan \beta \leq 750$ GeV. The results are further extrapolated at luminosities of 100 pb$^{-1}$ and 1000 pb$^{-1}$ for estimation of sensitivity in future LHC runs.

I. ACKNOWLEDGMENTS

The author would like to express his boundless gratitude to his supervisors Jan Steggemann and Andrew Gilbert for leading him all the way through the research and answering all his questions, being silly or not, in great detail. The author would like to thank Andrey Popov, Viola Sordini, Mauro Verzetti and Muhamand Gul for valuable discussions on the MG generation of signal and interference process, on matters concerning the $K$-factor and on the implementation of mass and width morphing algorithms. The author would also like to thank Luis Roberto Flores Castillo and Ming Chung Chu for their sincere help on general statistical methods and theory.

The author would like to acknowledge the department of physics at the Chinese University of Hong Kong and the CERN Summer Student Programme Committee for organizing the summer programme.
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