

Overcoming the challenges of quantum interference in Higgs physics with high-dimensional statistical inference















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Statistical inference methods developed for Higgs width You can follow technical details / intuitive explanations

What's to come



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Measuring quantum interference in the off-shell Higgs to flour leptons process with Machine Learning

Aishik Ghosh

Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France

Abstract — The traditional machine learning approach to optimize a particle physics measurement breaks down in the presence of quantum inference between the signal and background processes. A recently developed family of physics-aware machine learning techniques that rely on the extraction of additional information from the particle physics simulator to train the neural network could be adapted to a signal strength measurement problem. The networks are trained to directly learn the likelihood or likelihood ratio between the test hypothesis and null hypothesis values of the theory parameters being measured. We apply this idea to a signal strength measurement in the off-shell Higgs to four leptons analysis for the Vector Boson Fusion production mode from simulations of the high energy proton-proton collisions at the Large Hadron Collider. Promising initial results indicate that a model trained on simulated data at different values of the signal strength outperforms traditional approaches in the presence of quantum interference.

1 Introduction





(a) Signal: Higgs from Vector Boson Fusion

(b) Background: Vector Boson Scattering

Figure 1: Feynman Diagrams of the processes under study, (a) signal Higgs diagram, (b) interfering background diagram

The Heisenberg uncertainty principle of quantum mechanics $(\sigma_E \sigma_t \geq \frac{\hbar}{2})$ allows particles to become "virtual", with a mass going far away from the one described by special relativity's mass-energy equivalence formula $\tilde{E}^2 - |\vec{p}|^2 c^2 = m_0^2 c^4$ (where the energy E is given in terms of the rest mass m_0 and momentum \vec{p} of the particle and c is the speed of light in vacuum). They and are referred to as "off-shell" particles. Quar tum mechanics also prescribes that given an initial and final state, all possible intermediate states can and will occur, and they may interfere with one another.

A study of the off-shell Higgs boson decaying to two Z bosons that decay to four leptons (henceforth referred to as "offshell h4l"), such the 2018 study [2] in the AT-LAS Collaboration [1] is one of the most interesting studies in high energy particle physics because it allows to break certain degeneracies between the Higgs couplings, and constrain the Higgs width (under certain model dependent assumptions) that cannot be disentangled by an on-shell measurement alone. An update to the previous ATLAS study using the entire Run2 data will have develop innovative methodology to deal with quantum interference between the Higgs Feynman diagram (referred to as "signal") and other standard model processes (referred to as "background"). While the previous round used simple cuts to define the region of interest, we investigate a recently developed family of physics-aware machine learning techniques to improve the sensitivity of such an analysis. The two main diagrams studied here are shown in Figure 1. Other signal and background processes will be included in future studies. The objective of the analysis is to measure the "signal strength", μ , of the signal, which is a proxy for measuring how strongly the Higgs interacts with other fields. Interestingly, the usual notion that the signal strength corresponds to the ratio of the observed in data to the expected in Monte Carlo simulation signal yield breaks down in the presence of quantum interfer-

This study is performed with data simulated with MadGraph5_aMC [3], Pythia 8 [4] and Delphes 3 [5].

2 Machine Learning in a signal strength measurement

Traditionally, in analyses without quantum interference, one can train a machine learning classifier (such as a Boosted Decision Tree) to separate the signal and background samples (referred to as "events") that are simulated separately, and under the assumption that it is an optimal classifier, due to the Neyman-Pearson lemma [6], one can get the likelihood ratio [7] between a test hypothesis and the null hypothesis from the output of the classifier. The output of the classifier can be used for a fit to measure the signal strength, μ , optimally. In the presence of quantum interference, this strategy is no longer optimal. Figure 2 shows how a physics variable (the invariant mass of the four leptons) that is

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ATLAS CONF Note ATLAS-CONF-2024-015

28th October 2024

An implementation of Neural Simulation-Based **Inference for Parameter Estimation in ATLAS**

The ATLAS Collaboration

Neural Simulation-Based Inference (NSBI) is a powerful class of machine learning (ML)-based methods for statistical inference that naturally handles high-dimensional parameter estimation without the need to bin data into low-dimensional summary histograms. Such methods are promising for a range of measurements, including at the Large Hadron Collider (LHC), where no single observable may be optimal to scan over the entire theoretical phase space under consideration, or where binning data into histograms could result in a loss of sensitivity. This work develops an NSBI framework for statistical inference, using neural networks to estimate probability density ratios, which enables the application of NSBI to a full-scale LHC analysis. It incorporates a large number of systematic uncertainties, quantifies the uncertainty coming from finite training statistics, develops a method to construct confidence intervals, and demonstrates a series of intermediate diagnostic checks that can be performed to validate the robustness of the method. As an example, the power and feasibility of the method are demonstrated on simulated data for a simplified version of an off-shell Higgs boson couplings measurement in the four-leptons final states. This NSBI framework is an extension of the standard statistical framework used by LHC experiments and can benefit a large number of physics analyses.

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Measurement of off-shell Higgs boson production in the $H^* \rightarrow ZZ \rightarrow 4\ell$ decay channel using a neural simulation-based inference technique with the ATLAS detector at $\sqrt{s} = 13$ TeV

The ATLAS Collaboration

A measurement of off-shell Higgs boson production in the $H^* \rightarrow ZZ \rightarrow 4\ell$ decay channel is presented. The measurement uses the 140 fb^{-1} of integrated luminosity collected by the ATLAS detector during the Run 2 proton-proton collisions of the Large Hadron Collider at $\sqrt{s} = 13$ TeV and supersedes our previous result in this decay channel using the same dataset. The data analysis is performed using a neural simulation based-inference method, which builds per-event likelihood ratios using neural networks. The observed (expected) off-shell Higgs boson production signal strength in the $ZZ \rightarrow 4\ell$ decay channel is $0.87^{+0.75}_{-0.54}$ (1.00^{+1.04}) at 68% CL. The previous result was not able to achieve expected sensitivity to quote a two-sided interval at this CL. The expected plus-side uncertainty is reduced by 10%. The evidence for off-shell Higgs boson production has an observed (expected) significance of 2.5σ (1.3 σ) using the $ZZ \rightarrow 4\ell$ decay channel only. The expected significance score is 2.6 times that of our previous result using the same dataset. When combined with our most recent measurement in $ZZ \rightarrow 2\ell 2\nu$ decay channel, the evidence for off-shell Higgs boson production has an observed (expected) significance of 3.7σ (2.4 σ). The off-shell measurements are combined with the measurement of on-shell Higgs boson production to obtain constraints on the Higgs boson total width. The observed (expected) value of the Higgs boson width is $4.3^{+2.7}_{-1.0}$ ($4.1^{+3.5}_{-3.4}$) MeV



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The ATLAS Collaboration

Similar story for neutron star astrophysics

ournal of Cosmology and Astroparticle Physics An IOP and SISSA journal

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Neural simulation-based inference of the neutron star equation of state directly from telescope spectra

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ABSTRACT: Neutron stars provide a unique opportunity to study strongly interacting matter under extreme density conditions. The intricacies of matter inside neutron stars and their equation of state are not directly visible, but determine bulk properties, such as mass and radius, which affect the star's thermal X-ray emissions. However, the telescope spectra of these emissions are also affected by the stellar distance, hydrogen column, and effective surface temperature, which are not always well-constrained. Uncertainties on these nuisance parameters must be accounted for when making a robust estimation of the equation of state In this study, we develop a novel methodology that, for the first time, can infer the full posterior distribution of both the equation of state and nuisance parameters directly from

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https://doi.org/10.1088/1475-7516/2024/09/009











Some of the oldest questions



Image: <u>Source</u>

How sure are we? Theory of Errors & Empirical Knowledge (6 century BCE)

What elements make up the universe? (5 century BCE)



Volume II





Some of the oldest questions



Image: <u>Source</u>

How sure are we? Theory of Errors & Empirical Knowledge (6 century BCE)

What elements make up the universe? (5 century BCE)

Theorists





Volume II







Some of the oldest questions



Image: <u>Source</u>



Experimentalists

How sure are we? Theory of Errors & Empirical Knowledge (6 century BCE)

What elements make up the universe? (5 century BCE)

Theorists





Volume II









There's so much more dark matter than visible matter in the universe. What is it ?





There's so much more dark matter than visible matter in the universe. What is it ?



Image: GANIL



Why more matter than anti-matter ?



There's so much more dark matter than visible matter in the universe. What is it ?



Image: GANIL

Are there new forces ?



Why more matter than anti-matter ?



There's so much more dark matter than visible matter in the universe. What is it ?



Image: GANIL

Are there new forces ?

New theories often predict new particles yet to be discovered



Why more matter than anti-matter ?



















Protons are made up of u and d

That's the electron and it's cousins



Leptons









Protons are made up of u and d

That's the electron and it's cousins



Leptons









Protons are made up of u and d

That's the electron and it's cousins



Leptons





ACCELERATING SCIENCE



Heaver particles, difficult to create





That's the electron and it's cousins



Leptons



Higgs boson

Higgs field gives other particles mass





ACCELERATING SCIENCE



Smash particles at Large Hadron Collider





Smash particles at Large Hadron Collider





Smash particles at Large Hadron Collider



https://www.pinterest.es/pin/616148792741667669/





The detectors



The detectors

- Detector has O(100 million) sensors
- Can't build 100M dimensional histogram
- Reconstruction pipeline, event selection
- Design sensitive one-dimensional observable

Summarise in low dimensions





- Detector has O(100 million) sensors
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Summarise in low dimensions







Probability Density Estimation: What we're used to doing.











Probability Density Estimation: What we're used to doing.



Measure signal strength μ

With histograms we can ask "Given the data, what is the likelihood of $\mu = 1$ hypothesis vs $\mu = 2$ hypothesis?"







Probability Density Estimation: What we're used to doing.



Measure signal strength μ

With histograms we can ask "Given the data, what is the likelihood of $\mu = 1$ hypothesis vs $\mu = 2$ hypothesis?"





(Frequentist) Hypothesis tests





(Frequentist) Hypothesis tests

$\mathcal{L}(H_1 | data) = p(data | H_1)$







A measurement of the Higgs width





Undiscovered massive particles





- Enables the probe of a wide variety of new massive lacksquareparticles, other new physics
- Central topic for future colliders ullet





Undiscovered massive particles

A measurement of the Higgs width



New challenge: Quantum interference Non-linear changes in kinematics



Data can no longer be summarised in 1D histogram (see Ghosh et al: hal-02971995(p172))!


New challenge: Quantum interference Non-linear changes in kinematics



Data can no longer be summarised in 1D histogram (see Ghosh et al: hal-02971995(p172))!



















1-D projection

Theory 2



1-D projection

Theory 3

Theory 2



1-D projection

Theory 3

Theory 2



1-D projection

Theory 3

- Clearly separable in 2-D
- Theory 2 • No 1-D summary statistic may contain all the information needed to optimally test all theory hypotheses!
 - Valuable to have high-dimensional view of data

No single observable captures all information in Higgs width study

Signal-background-inference simulations: MG + Pythia

hal-02971995v3 (p172): Aishik Ghosh, David Rousseau









Optimal observable now changes as a function of **µ**: Cannot collapse problem to 1 dimension

hal-0297199512 (p172): Aishik Ghosh, David Rousseau

But probability density estimation in higher dimensions is hard...



1-D histogram with 6 bins: few events enough to populate it







But probability density estimation in higher dimensions is hard...



1-D histogram with 6 bins: few events enough to populate it

Curse of dimensionality

How many events for 50-D histogram with 6^{50} bins ?









High-dim data

<u>Neural simulation-based inference framework:</u>



Cranmer et al: <u>arXiv:1506.02169</u>

Traditional framework:

 μ is now arbitrary parameter of interest(s)









High-dim data

<u>Neural simulation-based inference framework:</u>



Cranmer et al: <u>arXiv:1506.02169</u>

Traditional framework:

Hypothesis μ_1 μ is now arbitrary parameter of interest(s)







<u>Neural simulation-based inference framework:</u>



Cranmer et al: <u>arXiv:1506.02169</u>







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NSBI for Higgs width in proof-of-concept phenomenology study



(Beyond Standard Model value)

hal-02971995v3 (p172): Aishik Ghosh, David Rousseau



NSBI for Higgs width in proof-of-concept phenomenology study



(Beyond Standard Model value) $\mu = 4$, without rate

NSBI for Higgs width in proof-of-concept phenomenology study



(Beyond Standard Model value) $\mu = 4$, without rate

Expected improvement for Standard Model



SM, wut



Open problems to extend to full ATLAS analysis:

- Robustness: Design and validation
- Systematic Uncertainties: Incorporate them in likelihood (ratio) model
- Neyman Construction: Throwing toys in a per-event analysis



Solved!

Open problems to extend to full ATLAS analysis:



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Solved!

Open problems to extend to full ATLAS analysis:

Applied on Runz data, superseding previous ATLAS paper on same data!

Presented at CHEP 2024, Higgs 2024



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Measurement of off-shell Higgs boson production in the $H^* \rightarrow ZZ \rightarrow 4\ell$ decay channel using a neural simulation-based inference technique with the ATLAS detector at $\sqrt{s} = 13$ TeV

The ATLAS Collaboration

A measurement of off-shell Higgs boson production in the $H^* \to ZZ \to 4\ell$ decay channel is presented. The measurement uses the 140 fb^{-1} of integrated luminosity collected by the ATLAS detector during the Run 2 proton-proton collisions of the Large Hadron Collider at $\sqrt{s} = 13$ TeV and supersedes our previous result in this decay channel using the same dataset. The data analysis is performed using a neural simulation based-inference method, which builds per-event likelihood ratios using neural networks. The observed (expected) off-shell Higgs boson production signal strength in the $ZZ \rightarrow 4\ell$ decay channel is $0.87^{+0.75}_{-0.54}$ $(1.00^{+1.04}_{-0.95})$ at 68% CL. The previous result was not able to achieve expected sensitivity to quote a two-sided interval at this CL. The expected plus-side uncertainty is reduced by 10%. The evidence for off-shell Higgs boson production has an observed (expected) significance of 2.5σ (1.3 σ) using the $ZZ \rightarrow 4\ell$ decay channel only. The expected significance score is 2.6 times that of our previous result using the same dataset. When combined with our most recent measurement in $ZZ \rightarrow 2\ell 2\nu$ decay channel, the evidence for off-shell Higgs boson production has an observed (expected) significance of 3.7σ (2.4 σ). The off-shell measurements are combined with the measurement of on-shell Higgs boson production to obtain constraints on the Higgs boson total width. The observed (expected) value of the Higgs boson width is $4.3^{+2.7}_{-1.9}$ ($4.1^{+3.5}_{-3.4}$) MeV at 68% CL.

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O(16) observables









Networks adjust likelihood for each systematic uncertainty







Networks adjust likelihood for each systematic uncertainty









- + Train $O(10^4)$ networks on TensorFlow
- ✦ Fits with JAX

Networks adjust likelihood for each systematic uncertainty

+ Computing resources provided by Google, SMU, other HPC clusters







Open problems to extend to full ATLAS analysis:

- Robustness: Design and validation
- Systematic Uncertainties: Incorporate them in likelihood (ratio) model
- Neyman Construction: Throwing toys in a per-event analysis

Next 2 slides gets a bit technical



$$x_i$$
 is one individual event Gen $p(x_i|\mu) = \frac{1}{\nu(\mu)} \sum_{j=1}^{C} f_j(\mu) \cdot \nu_j \ p_j(x_i)$



eral Formula

j runs over different physics process (Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)

Example use case







$$x_i$$
 is one individual event Gen $p(x_i|\mu) = \frac{1}{\nu(\mu)} \sum_{j=1}^{C} f_j(\mu) \cdot \nu_j \ p_j(x_i)$

$$p_{ggF}(x|\mu) = \frac{1}{\nu_{ggF}(\mu)} \left[\left(\mu - \sqrt{\mu}\right) \nu_S p_S(x) + \frac{1}{\nu_{ggF}(\mu)} \right]$$

neral Formula

j runs over different physics process (Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)

nple use case







$$\begin{aligned} x_i \text{ is one individual event} & \text{Gen}_i \\ p(x_i|\mu) &= \frac{1}{\nu(\mu)} \sum_{j=1}^{C} f_j(\mu) \cdot \nu_j \ p_j(x_i) \\ & \text{Comes from} \\ \\ p_{\text{ggF}}(x|\mu) &= \frac{1}{\nu_{\text{ggF}}(\mu)} \left[(\mu - \sqrt{\mu}) \ \nu_S \ p_S(x) + \frac{1}{\sqrt{2}} \right] \end{aligned}$$

eral Formula

j runs over different physics process (Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)

m theory model chosen to interpret data

nple use case









$${}_{gF}(x|\mu) = \frac{1}{\nu_{ggF}(\mu)} \left[(\mu - \sqrt{\mu}) \nu_{S} p_{S}(x) + \right]$$

General Formula

j runs over different physics process (Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)

Comes from theory model chosen to interpret data

Example use case









$$p_{ggF}(x|\mu) = \frac{1}{\nu_{ggF}(\mu)} \left[(\mu - \sqrt{\mu}) \nu_{S} p_{S}(x) + \sqrt{\mu} \right]$$

ral Formula
?
j runs over different physics proce (Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow$
n theory model chosen to interpret data
ole use case
$\sqrt{\mu} v_{\text{SBI}_1} p_{\text{SBI}_1}(x) + (1 - \sqrt{\mu}) v_{\text{B}} p_{\text{B}}(x)$









$$p_{ggF}(x|\mu) = \frac{1}{\nu_{ggF}(\mu)} \left[(\mu - \sqrt{\mu}) \nu_{S} p_{S}(x) + \right]$$







$$(\mu - \sqrt{\mu}) v_{S} + \sqrt{\mu} v_{SBI_{1}} \frac{p_{SBI_{1}}(x)}{p_{S}(x)} + (1 - \sqrt{\mu}) v_{B} \frac{p_{B}}{p_{S}}$$




Search-Oriented Mixture Model



Peral Formula
Estimated using an ensemble of network

$$p(x_i|\mu) = \frac{1}{v(\mu)} \sum_{j}^{C} f_j(\mu) \cdot v_j \frac{p_j(x_i)}{p_{ref}(x_i)}$$

erence hypothesis j runs over different physics proce
(Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow decomposition)$
m theory model chosen to interpret data
ple use case
 $\sqrt{\mu} v_{SBI_1} p_{SBI_1}(x) + (1 - \sqrt{\mu})v_B p_B(x)$

$$\mu - \sqrt{\mu} v_{S} + \sqrt{\mu} v_{SBI_{1}} \frac{p_{SBI_{1}}(x)}{p_{S}(x)} + (1 - \sqrt{\mu}) v_{B} \frac{p_{B}}{p_{S}}$$











 $\frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{\nu(\mu)} \sum_{i}^{C} f_j(\mu) \cdot \nu_j \frac{p_j(x_i)}{p_{\text{ref}}(x_i)}$

A separate classifier per physics process j (Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)







$$\frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{\nu(\mu)} \sum_{j=1}^{C} f_j(\mu) \cdot \nu_j \frac{p_j(x_j)}{p_{\text{ref}}(x_j)}$$

A separate classifier per physics process j (Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)







$$\frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{\nu(\mu)} \sum_{j=1}^{C} f_j(\mu) \cdot \nu_j \frac{p_j(x_j)}{p_{\text{ref}}(x_j)}$$

(Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)





$$\frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{\nu(\mu)} \sum_{j=1}^{C} f_j(\mu) \cdot \nu_j \frac{p_j(x_j)}{p_{\text{ref}}(x_j)}$$



$$\frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{\nu(\mu)} \sum_{j=1}^{C} f_j(\mu) \cdot \nu_j \frac{p_j(x_j)}{p_{\text{ref}}(x_j)}$$

Open problems to extend to full ATLAS analysis:

- Robustness: Design and validation
- Systematic Uncertainties: Incorporate them in likelihood (ratio) model • Neyman Construction: Throwing toys in a per-event analysis



Validate quality of LR estimation with re-weighting task

Reweighting: Calculate weights w_i for events x_i in blue sample to match green sample





Reweighting: Calculate weights w_i for events x_i in blue sample to match green sample

$$w_{i} = r(x_{i}, \mu_{0}, \mu_{1}) = \frac{p(x_{i} | \mu_{0})}{p(x_{i} | \mu_{1})}$$

Already estimated using an ensemble of networks

Validate quality of LR estimation with re-weighting task







Calibration curves of probability density ratios

 $\frac{p_{\mu=0.3}(x_i)}{p_{ref}(x_i)}$



Ensemble prediction









No bias: Method recovers correct value of μ on average

(Correct value when tested on the median 'Asimov dataset')

And many more diagnostics (see <u>backup</u>)

2.5



Open problems to extend to full ATLAS analysis: ✓ Robustness: Design and validation

- Systematic Uncertainties: Incorporate them in likelihood (ratio) model • Neyman Construction: Throwing toys in a per-event analysis



Systematic uncertainties



Image: arXiv:2105.08742





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Systematic uncertainties



• We only have simulations at 3 variations of each nuisance parameter α_k





Known interpolation strategies

See formula used in backup



⇒ Combine these traditional interpolation with neural network estimation of per-event likelihood ratios





 x_i is one individual event

 $\frac{p(x_i \mid \mu, \underline{\alpha})}{p_{ref}(x_i)} =$

See details of vertical interpolation for $G_j(\alpha_k), g_j(x_i, \alpha_k)$





 x_i is one individual event

 $\frac{p(x_i \mid \mu, \underline{\alpha})}{p_{ref}(x_i)} = \frac{1}{\nu(\mu, \alpha)} \sum_{i=1}^{C} f_j(\mu) \cdot \nu_j \cdot \frac{p_j(x_i)}{p_{ref}(x_i)} \cdot \prod_{k=1}^{N_{syst}} G_j(\alpha_k) \cdot g_j(x_i, \alpha_k)$

See details of vertical interpolation for $G_j(\alpha_k), g_j(x_i, \alpha_k)$





 $\frac{p(x_i \mid \mu, \underline{\alpha})}{p_{ref}(x_i)} = \frac{1}{\nu(\mu, \alpha)} \sum_{j=1}^{C} \frac{1}{p_{ref}(x_i)} \sum_{j=1}^{D$

See details of vertical interpolation for $G_j(\alpha_k), g_j(x_i, \alpha_k)$

 $\frac{p(x_i \mid \mu, \underline{\alpha})}{p_{ref}(x_i)} = \frac{1}{\nu(\mu, \alpha)} \sum_{j=1}^{C} f_j(\mu) \cdot \nu_j \cdot \frac{p_j(x_i)}{p_{ref}(x_i)} \prod_{k=1}^{N_{syst}} G_j(\alpha_k) \cdot g_j(x_i, \alpha_k)$

We have this already





 x_i is one individual event N_{syst} $\int f_j(\mu) \cdot \nu_j \cdot \frac{p_j(x_i)}{1-2}$ $\cdot \frac{f}{p_{ref}(x_i)} \cdot \int \int G_j(\alpha_k) \cdot g_j(x_i, \alpha_k)$ $p(x_i | \mu, \underline{\alpha})$ $p_{ref}(x_i)$ $\nu(\mu, \alpha)$ We have this already $g_j(x_i, \alpha_k) = \frac{p_j(x_i, \alpha_k)}{p_i(x_i)}$ α_2 Estimate from simulations and existing α_1 interpolation methods

See details of vertical interpolation for $G_i(\alpha_k), g_i(x_i, \alpha_k)$



 x_i is one individual event $\sum_{j=1}^{N} f_j(\mu) \cdot \nu_j \cdot \frac{p_j(x_i)}{p_{ref}(x_i)} \prod_{l=1}^{N_{syst}} G_j(\alpha_k) \left(g_j(x_i, \alpha_k) \right)$ $p(x_i | \mu, \underline{\alpha})$ $p_{ref}(x_i)$ $\nu(\mu, \alpha)$ We have this already Per-event terms estimated using another ensemble of networks and interpolation methods $g_j(x_i, \alpha_k) = \frac{p_j(x_i, \alpha_k)}{p_j(x_i)}$ α_2 Estimate from simulations and existing α_1 interpolation methods

See details of vertical interpolation for $G_i(\alpha_k), g_i(x_i, \alpha_k)$







$\begin{aligned} x_i \text{ is one individual event} \\ \frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \end{aligned}$

$$\prod_{i}^{N_{\text{data}}} \frac{p(x_i|\mu,\alpha)}{p_{\text{ref}}(x_i)} \prod_{k} \text{Gaus}(a_k|\alpha_k,\delta_k)$$



x_i is one individual event





 x_i is one individual event $\frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \prod_{i}^{N_{\text{data}}} \frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)}$





Prod over events



















Non-parabolic shape due to non-linear effects from quantum interference

Reference Sample

A combination of signal samples, to ensure there's non-vanishing support entire region of analysis Does not have to be physical!

$$p_{\text{ref}}(x_i) = \frac{1}{\sum_k v_k} \sum_{k=1}^{C_{\text{signals}}} v_k \cdot p_k(x_i)$$

$$\Rightarrow \text{ In our dataset, } p_{ref}(\cdot) = p_S(\cdot)$$

Choice of $p_{ref}(\cdot)$ can be made purely on numerical stability of training, as it drops out in profile step

$$t_{\mu} = -2\ln\left(\frac{L_{\text{full}}(\mu,\widehat{\hat{\alpha}})/\mathcal{L}_{\text{ref}}}{L_{\text{full}}(\widehat{\mu},\widehat{\alpha})/\mathcal{L}_{\text{ref}}}\right)$$



Open problems to extend to full ATLAS analysis:

- ✓ Robustness: Design and validation
- ✓ Systematic Uncertainties: Incorporate them in likelihood (ratio) model
- Neyman Construction: Throwing toys in a per-event analysis



Traditionally:



What if events have negative weights? See backup

Throwing event-level toys

NSBI:



$$w_i^{toy} = Poisson(w_i^{Asimov})$$

('Unweighted' events, i.e. integer weights)





Confidence belts



-Similar to structure seen in histogram analysis



Why does NSBI work better than traditional analyses?



Why does it work better than traditional analyses?





Why does it work better than traditional analyses?



Significant improvement in QI impacted region





Significant improvement in QI impacted region

O_{fixed} = log
$$\frac{p_{S}(x_{i})}{p_{SBI}(x_{i})}$$
: Similar to histogram analysis
 $O_{\mu} = \frac{p(x_{i} | \mu)}{p(x_{i} | \mu = 1)}$: Parameterised observable, histogram analysis
NSBI: Parameterised, unbinned
 O_{μ} approaches NSBI as nBins → ∞
2.5




NSBI vs histogram analysis



Observed data happens to provide stronger than expected constrains for both hist and NSBI (consistent)

Results on data

Stat vs Stat+Syst



Nuisance parameters decrease sensitivity, as expected









Image: <u>Source</u>







Telescope measurements of energy spectra of neutron stars



Figure from Lattimer J. M., Prakash M., 2001, The Astrophysical Journal, 550, 426–442

Mass-radius curves created by different equation of state (EoS) models

Horizontal bars show massive neutron star observations used to "rule out" EoS models.

Two communities:

- Astrophysicists measure mass/radius from telescope
- Nuclear theorists measure EoS from mass/radius







Telescope measurements of energy spectra



Radius

Effective Temperature



Traditional method: Two-step inference



JCAP.020P.0922: Delaney Farrell, Pierre Baldi, Jordan Ott, Aishik Ghosh, Andrew W. Steiner, Atharva Kavitkar, Lee Lindblom, Daniel Whiteson, Fridolin Weber



Traditional method: Two-step inference



Leak some information on uncertainties in the handover

JCAP.020P.0922: Delaney Farrell, Pierre Baldi, Jordan Ott, Aishik Ghosh, Andrew W. Steiner, Atharva Kavitkar, Lee Lindblom, Daniel Whiteson, Fridolin Weber



Traditional method: Two-step inference



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Inferring neutron star EoS parameters with NSBI

Recover the likelihood of EoS + NPs directly from the raw high-dimensional telescope spectra!



Neutron star in sky

Astrophysicists



Direct estimation of likelihood from high-dimensional raw data allows more reliable uncertainty propagation and better measurements!

CAP09(2024)009: Brandes, Modi, Ghosh, et al

JCAP12(2023)022: Farrell, Baldi, Ott, Ghosh, et al

Nuclear physicists

JCAP02(2023)016: Farrell, Baldi, Ott, **Ghosh**, et al 48



Meaningful posteriors, most sensitive method !



Bayesian Posteriors and credible intervals





Prior knowledge on nuisance parameters

Only possible to visualise these due to the fast and differentiable likelihood from networks





- Quantum interference breaks assumptions in traditional statistical methods at LHC
- Neural inference can optimally handle these challenges for Higgs width:
 - Shown in phenomenology study
 - Developed method for deployment in ATLAS
 - Re-analysed Run 2 data and achieved a dramatic improvement in sensitivity $(H \rightarrow 4l)$
- NSBI has wide-ranging applications, in particle physics, astrophysics and beyond!
- Weaknesses: Same as traditional analyses (systematics, training statistics). Developed diagnostic tools to help







Thanks !

Reach out: Email



for which the weaker assumption shell, shell shell, shell s scale factors, the factors, the ratio of unit and been broken by the house of the Hission. This assumption is bartly $gg \rightarrow t Hale planet then$ be probed in the second of the With the current wants and the ftor state g While the here the off beck signal and the second of the se highersenting the state of the second states and the second states leading order a contraction of the state of background joe Bunnie Building of the second sensitive to the jet multiplicity ent selse in the test in the production which is the dependence on the boost of the VV system, which is















Choice of observable



Choice of observable

Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods:



 $\mathcal{L}(\mu \,|\, \mathcal{D}) = p(\mathcal{D} \,|\, \mu)$





Choice of observable

Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods:

 $p(\mathcal{D} \mid \mu)$ $p(\mathcal{D} \mid \mu_0)$ $\mathcal{L}(\mu \,|\, \mathcal{D}) = p(\mathcal{D} \,|\, \mu)$





Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods:



A neural network classifier trained on S vs B, estimates the decision function*:

* Equal class weights

Choice of observable

 $\mathscr{L}(\mu \mid \mathscr{D}) = p(\mathscr{D} \mid \mu)$

 $s(x_i) = \frac{p(x_i \mid S)}{p(x_i \mid S) + p(x_i \mid B)}$





Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic $p(\mathcal{D} \mid \mu)$ We want to compare likelihoods: $p(\mathcal{D} \mid \mu_0)$

 $s(x_i) = \frac{p(x_i \mid S)}{p(x_i \mid S) + p(x_i \mid B)}$ A neural network classifier trained on S vs B, estimates the decision function*:

Which contains all the information required for the likelihood ratio:

$$\frac{p(x_i \mid \mu)}{p(x_i \mid \mu = 0)} = \frac{1}{\mu \cdot \nu_S + \nu_B} \frac{\mu \cdot \nu_S p(x_i \mid \mu = 0)}{\mu \cdot \nu_S + \nu_B}$$

Same observable s is optimal to test all μ hypotheses! No need to develop separate analysis per hypothesis μ

* Equal class weights

Choice of observable

$$\mathscr{L}(\mu \,|\, \mathscr{D}) = p(\mathscr{D}$$

 $\frac{v_i | S) + \nu_B p(x_i | B)}{p(x_i | B)} = \frac{\mu}{\mu \cdot \nu_S + \nu_B} \cdot \frac{s(x_i)}{1 - s(x_i)} + \nu_B$











Estimating high-dimensional density ratios

Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods:

 $\frac{p(\mathcal{D} \mid \mu)}{p(\mathcal{D} \mid ref)}$

A neural network classifier trained on simulated samples from θ_1 vs simulated samples from *ref*, estimates the decision function:

Which contains all the information required for the likelihood ratio:

p(]

* Optimal statistic to test each value of μ * We get the LR *per event (*unbinned)

 $\mathscr{L}(\mu \,|\, \mathscr{D}) = p(\mathscr{D} \,|\, \mu)$

 $s(x_i) = \frac{p(x_i | \mu_1)}{p(x_i | \mu_1) + p(x_i | ref)}$

$$\frac{(x_i | \mu_1)}{x_i | ref} = \frac{s(x_i)}{1 - s(x_i)}$$







More diagnostics







Interpretability: Which phase space favours one hypothesis over another?

$$-2 \cdot log \frac{P(x_i | \mu = 0.5)}{P(x_i | \mu = 1)}$$



$$-2 \cdot log \frac{P(x_i | \mu = 1.5)}{P(x_i | \mu = 1)}$$





NN observable



Data-MC validation





Data-MC validation

Different NN observables









Neyman construction



Neyman Construction

- To build confidence intervals, we need to 'invert the hypothesis test'





• Generate pseudo-experiments ('toys') and determine 1σ & 2σ CI as a function of parameter of interest



Negative Weighted Events

- 1. Start from a positive weighted reference sample instead
- 2. Re-weight to intended parameter point
- 3. Throw toys from this sample

$$w_i^{\text{rwt-ref}} \to w_i^{\text{Asimov}}(\mu, \alpha) =$$

 $= \frac{v(\mu, \alpha)}{v_{\text{rwt-ref}}} \cdot \frac{p(x_i | \mu, \alpha)}{p_{\text{rwt-ref}}(x_i)} \cdot w_i^{\text{rwt-ref}}$



Uncertainty from finite training samples



Estimating the variance on mean: Bootstrapping



Image: <u>Source</u>

the mean



$$w_i \rightarrow w_i \cdot Pois(1)$$

- Train an ensemble of networks, each on a Poisson fluctuated version of the training dataset
- Ensemble average used as final prediction, estimate the variance on \bullet mean from bootstrapped ensembles

Quantifying uncertainty on estimated density ratio





$$w_i \rightarrow w_i \cdot Pois(1)$$

- Train an ensemble of networks, each on a Poisson fluctuated version of the training dataset
- Ensemble average used as final prediction, estimate the variance on lacksquaremean from bootstrapped ensembles

Quantifying uncertainty on estimated density ratio

INPU Neural Network #2 Neural Network #3 Neural Network #1 Ensemble OUTPUT




$$w_i \rightarrow w_i \cdot Pois(1)$$

- Train an ensemble of networks, each on a Poisson fluct the training dataset
- Ensemble average used as final prediction, estimate the variance on mean from bootstrapped ensembles



$$w_i \rightarrow w_i \cdot Pois(1)$$

- Train an ensemble of networks, each on a Poisson fluct the training dataset
- Ensemble average used as final prediction, estimate the variance on mean from bootstrapped ensembles
- Propagate with spurious signal method

 $f_j(\mu) \to f_j(\mu + \alpha \cdot \Delta \hat{\mu}(\mu))$

Constraint term: Gauss(0,1)



Combination with histogram analyses

 $\frac{L_{\text{comb}}(\mu, \alpha)}{L_{\text{ref}}} = \frac{L_{\text{full}}(\mu, \alpha)}{L_{\text{ref}}} L_{\text{hist}}(\mu, \alpha)$



Calculating pulls and impacts in JAX

Hessian:

$$C_{nm} = \left[\frac{1}{2} \frac{\partial^2 \lambda}{\partial \alpha_n \partial \alpha_m}(\hat{\mu}, \hat{\alpha})\right]^{-2}$$

Pulls:

 $\frac{\widehat{\alpha}_k - \alpha_k^0}{\sqrt{C_{kk}}}.$

Post-fit Impact:

$$\Gamma_{k} = \frac{\partial \widehat{\mu}}{\partial \alpha_{k}} \times \sqrt{C_{kk}}$$
$$= -\left[\frac{\partial^{2} \lambda}{\partial^{2} \mu}(\widehat{\mu}, \widehat{\alpha})\right]^{-1} \frac{\partial^{2} \lambda}{\partial \mu \partial \alpha_{k}}(\widehat{\mu}, \widehat{\alpha}) \times \sqrt{C_{kk}},$$

$$\lambda(\mu, \alpha) = -2 \ln(L_{full}(\mu, \alpha)/L)$$





$$G_{j}(\alpha_{k}) = \begin{cases} \left(\frac{\nu_{j}(\alpha_{k}^{+})}{\nu_{j}(\alpha_{k}^{0})}\right)^{\alpha_{k}} & \alpha_{k} > 1\\ 1 + \sum_{n=1}^{6} c_{n}\alpha_{k}^{n} & -1 \le \alpha_{k} \le 1\\ \left(\frac{\nu_{j}(\alpha_{k}^{-})}{\nu_{j}(\alpha_{k}^{0})}\right)^{-\alpha_{k}} & \alpha_{k} < -1 \end{cases}$$

With some continuity requirements

Vertical interpolation

$$g_j(x_i, \alpha_k) = \begin{cases} \left(g_j(x_i, \alpha_k^+)\right)^{\alpha_k} & \alpha_k > 1\\ 1 + \sum_{n=1}^6 c_n \alpha_k^n & -1 \le \alpha_k \le 0\\ \left(g_j(x_i, \alpha_k^-)\right)^{-\alpha_k} & \alpha_k < -1 \end{cases}$$







Physics analysis results



Systematic Uncertainty Fixed

All (stat-only)

Parton shower uncertainty for $gg \rightarrow ZZ$ (nor Parton shower uncertainty for $gg \rightarrow ZZ$ (sha NLO EW uncertainty for $q\bar{q} \rightarrow ZZ$ NLO QCD uncertainty for $gg \rightarrow ZZ$ Parton shower uncertainty for $q\bar{q} \rightarrow ZZ$ (sha Jet energy scale and resolution uncertainty

None (full result)

	$\mu_{\text{off-shell}}$ Value at which $t_{\mu_{\text{off-shell}}} = 4$				
	NSBI analysis	Histogram-based			
	1.96	2.13			
rmalization)	2.07	2.26			
ape)	2.12	2.29			
	2.10	2.27			
	2.09	2.29			
ape)	2.12	2.29			
	2.11	2.26			
	2.12	2.30			



$$p(x|\mu_{\text{off-shell}}^{\text{ggF}}, \mu_{\text{off-shell}}^{\text{EW}}) = \frac{1}{\nu(\mu_{\text{off-shell}}^{\text{ggF}}, \mu_{\text{off-shell}}^{\text{EW}})} \times \left[\mu_{\text{off-shell}}^{\text{ggF}} \nu_{\text{S}}^{\text{ggF}} p_{\text{S}}^{\text{ggF}}(x) + \sqrt{\mu_{\text{off-shell}}^{\text{ggF}}} \nu_{\text{I}}^{\text{ggF}} p_{\text{I}}^{\text{ggF}}(x) + \nu_{\text{B}}^{\text{ggF}} p_{\text{B}}^{\text{ggF}}(x) + \mu_{\text{off-shell}}^{\text{EW}} \nu_{\text{S}}^{\text{EW}} p_{\text{S}}^{\text{EW}}(x) + \sqrt{\mu_{\text{off-shell}}^{\text{EW}}} \nu_{\text{I}}^{\text{EW}} p_{\text{I}}^{\text{ggF}}(x) + \nu_{\text{B}}^{\text{EW}} p_{\text{B}}^{\text{ggF}}(x) + \mu_{\text{NI}} p_{\text{NI}}(x) \right]$$

Variable	Definition				
$m_{4\ell}$	quadruplet mass				
m_{Z1}	Z_1 mass				
m_{Z2}	Z_2 mass				
$\cos heta^*$	cosine of the Higgs boson decay angle $[\mathbf{q}_1 \cdot \mathbf{n}_z / \mathbf{q}_1]$				
$\cos \theta_1$	cosine of the Z_1 decay angle $[-(\mathbf{q}_2) \cdot \mathbf{q}_{11}/(\mathbf{q}_2 \cdot \mathbf{q}_{11})]$				
$\cos \theta_2$	cosine of the Z ₂ decay angle $[-(\mathbf{q}_1) \cdot \mathbf{q}_{21}/(\mathbf{q}_1 \cdot \mathbf{q}_{21})$				
Φ_1	Z_1 decay plane angle $[\cos^{-1}(\mathbf{n}_1 \cdot \mathbf{n}_{sc}) (\mathbf{q}_1 \cdot (\mathbf{n}_1 \times \mathbf{n}_{sc})/(\mathbf{q}_1 \cdot$				
Φ	angle between Z_1, Z_2 decay planes $[\cos^{-1}(\mathbf{n}_1 \cdot \mathbf{n}_2) (\mathbf{q}_1 \cdot (\mathbf{n}_1 \times \mathbf{n}_2))/$				
$p_T^{4\ell}$	quadruplet transverse momentum				
$y^{4\ell}$	quadruplet rapidity				
n _{jets}	number of jets in the event				
m_{jj}	leading dijet system mass				
$\Delta \eta_{jj}$	leading dijet system pseudorapidity				
$\Delta \phi_{jj}$	leading dijet system azimuthal angle difference				

 $\left| \right) \right]$])] $|\mathbf{n}_1 \times \mathbf{n}_{sc}|)]$ $(|\mathbf{q}_1| \cdot |\mathbf{n}_1 \times \mathbf{n}_2|)]$















Traditionally ignoring systematic uncertainties during analysis optimisation

Experimental uncertainties: Eg. Inaccuracies in the calibration of our detector



PRD.104.056026: Aishik Ghosh, Benjamin Nachman, and Daniel Whiteson

- Current analyses strategies optimised while ignoring systematic uncertainties
- Added in post-facto
- Leads to loss in sensitivity compared to uncertaintyaware optimisation (see details)





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Difference b/w post-facto and uncertainty-aware

Traditionally ignoring systematic uncertainties during analysis optimisation

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Avoids binning data into histograms, which is another lossy compression









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$p(\text{theory} | \text{data}) = \frac{p(\text{data} | \text{theory})p(\text{theory})}{p(\text{data})}$



What we all want (Posterior)

 $p(\text{theory} | \text{data}) = \frac{p(\text{data} | \text{theory})p(\text{theory})}{p(\text{theory})}$

p(data)



What we all want (Posterior)

p(theory | data) = -



p(data)



What we all want (Posterior)

Likelihood Prior p(data | theory)p(theory) p(theory | data) =*p*(data)

Evidence





- Test potential improvement in sensitivity coming from new measurements
- Could inform decisions on which stars to measure next!



Most sensitive method for EoS inference to date!

NP priors			$\lambda_{1,\mathrm{pred}} - \lambda_{1,\mathrm{truth}}$		$\lambda_{2,\mathrm{pred}} - \lambda_{2,\mathrm{truth}}$		Combined
	p(u)	Method	μ	σ	μ	σ	$\sigma_{ m tot}$
Pretend that nuisance parameters known exactly	true	ML -Likelihood $_{EOS}$	-0.02	0.066	0.01	0.070	0.096
		NN(Spectra)	-0.02	0.066	0.01	0.075	0.099
		NN(M, R via XSPEC)	-0.03	0.065	0.01	0.055	0.085
		NLE	0.00	0.056	-0.01	0.070	0.090
	tight	ML-Likelihood EOS	-0.02	0.078	0.03	0.081	0.112
		NN(Spectra)	0.02	0.085	-0.02	0.077	0.115
		NN(M, R via XSPEC)	-0.03	0.081	0.01	0.056	0.098
Realistic scenarios: <		NLE	0.00	0.066	-0.02	0.071	0.097
	loose	ML -Likelihood $_{EOS}$	-0.04	0.089	0.03	0.081	0.120
		NN(Spectra)	-0.03	0.131	-0.01	0.078	0.152
		NN(M, R via XSPEC)	-0.03	0.123	0.01	0.058	0.136
		NLE	0.00	0.085	-0.01	0.074	0.113

