

Data Analysis in High-Energy Physics as a Differentiable Program

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Preface

“I didn’t have time to write a short letter thesis, so I wrote a long one instead.” —
Mark Twain (adapted)

Many curious things can stem from direct messages on Twitter(cite). You can count the contents of this thesis as one of them.

In October of 2019, I got off the tram from the Blandonnet stop in Geneva, arriving bewildered to CERN for a 6 month placement. I had no idea what I was going to be doing there, since my assigned supervisor and I had not communicated at any point leading up to this visit. I just knew that I was doing this placement as part of my position, which was funded as part of a Marie Curie International Training Network (they let you do placements), and that my supervisor was in some way connected to the team working on the ROOT software suite.

Now, ROOT is sometimes talked about with a negative tone in high-energy physics circles due to its steep learning curve and monolithic software design. I will endeavour to do no such thing here, as this software was a revolution in computing for its time, and continues to power the majority of data analysis done at the Large Hadron Collider. However, this is specialist software, and it is very much the case that the typical undergraduate/masters student will likely have no training on how to use it, which can significantly hinder the ability to play with your code and understand what’s going on. Moreover, many courses at university will be teaching students to have proficiency with more standard scientific analysis tools, such as the scientific Python ecosystem. Being one of these people, I was keen to explore to what extent I could utilize these tools that I had some familiarity with in order to do my physics work. This led to me tweeting out the below, a mere two months before my placement:

pyhf is being used in a few on-going projects within ATLAS, also people like e.g. uproot for ntuple analysis. Complete end-to-end is difficult since reading xAOD in uproot natively isn’t easy to achieve (also need C++ CP tools etc). I’m happy to help/collaborate!

— Lukas Heinrich ((lukasheinrich_?)) August 21, 2019

I enthusiastically followed up on Lukas’ offer to collaborate, and before I knew it, I was sat at a table in CERN’s main restaurant (R1 if you’re a cool kid) with both Lukas and my would-be supervisor (who would not be my supervisor), ready to start a project on building something that had never been done before, but using tools that I was familiar with. That project became **neos**, and started the development of a new paradigm for how we view optimizing our data analysis pipelines, and the cornerstone of this thesis – differentiable programming. Totally different from just a ROOT-less analysis, but I also did a bit of that in the end anyway.

As such, if you were expecting a typical HEP thesis, you may be surprised at what lies ahead, hopefully in a positive matter. We will still traverse the lands of particle physics, but will be stepping around many puddles that most dive into, and instead spend a bit of extra time in the marshlands of probability and statistics, which inform almost all of the work done in my PhD from a practical and motivational standpoint. From there, we'll foray into the fields of gradients, including how we calculate them, why we care, and what they're used for. There, we will meet the buzzwords that you may have come here for in the first place: **machine learning** and **differentiable programming**. Armed with these fundamentals, we will tackle my application of them to problems in collider physics, including optimizing summary statistics while being aware of uncertainty, interpolating between new physics models, and searching for new particles produced in association with a Higgs boson! (Maybe there's puppies too. I don't know. But don't you want to find out?)

This is a book created from markdown and executable code, thanks to the [Quarto framework](#).

Part I

Fundamentals

1 Physics background

What makes up you and me? How do interactions on the smallest scales affect the way the universe was made and how it will end? Why does anything exist at all? Is anyone even reading this? If they do, but no-one is there to see them, will they make a sound?

At least two of these existential questions are explored by the scientific discipline known as **high-energy physics** (HEP). This term encompasses things like **particle physics**, **astrophysics**, and **cosmology**, which are a mix of studying things at the largest and smallest possible scales, and have surprisingly large interplay. We focus here on particle physics, which looks at the very, very small.

An innumerable number of particle physics results in the last 10 years or so have shown no signs of deviating from the predictions made from the **Standard Model** of particle physics, a theory proposed and developed by many scientists over many years (Oerter 2006). It's been extraordinarily robust to experiments that have probed it thus far, and it is very much the norm for any budding physicist to pessimistically assume any search to uncover new physics will state "no excesses were found", with the result being "consistent with the Standard Model prediction". We go over an extremely brief overview of this ludicrously successful model in the following paragraphs, which are largely based on (Tong 2022) and (Buckley, White, and White 2021).

The Standard Model is a type of **quantum field theory**, which operates using a fundamental object defined over all of time and space called a *field*. These fields are described by equations that can be treated as waves, which are restricted to travel in discrete quanta of energy. These quanta are generally what we've been calling "particles", and also serve to mediate what we know as **forces**. Said in another way, everything that we call a particle is actually an oscillation of a field, where the field is the fundamental object as opposed to the particle. Nevertheless, the following conversation is mostly had from a particle-first perspective in order to salvage some intuition, even if it breaks down under a fine enough microscope (somewhat literally – we'll get to this in due course). So, even though we won't mention them too much, do keep in the back of your mind that everything that manifests here is actually a result of these fields interacting in some way¹.

Now, as far as I have checked, I am particles. So are you. Which particles are we? Textbooks would have us believe that we're made of "atoms", which in turn are made up of protons,

¹One cool thing I discovered while writing this thesis from David Tong's lecture notes is the following: the fact two particles of the same type have all the same properties can be thought of as two people putting their hand in a big sandpit and sculpting a particle from the a handful of sand.

neutrons, and electrons. Are they made up of their own “atoms” too? In a sense; the electron is irreducible as far as we know, but protons and neutrons are composed of constituents known as **quarks**, which again, don’t seem to be further reducible (at least from the perspective of the Standard Model). These quarks come in two “flavors”: the *up quark* u and the *down quark* d . There’s no particular reason for these names other than to make it neat to tell apart quarks in a linguistically pleasing way. Zooming out again to an atomic scale, the proton has a quark composition of uud (two up quarks and one down quark), and a neutron has udd (two down, one up)².

One last ingredient we’ll add here to complete this set of particles is the **neutrino**: an electrically neutral particle with extremely low mass. How do we even know it exists if it doesn’t noticeably interact with electromagnetic or gravitational forces? While not responsible for building up matter like me and you, it plays a role when matter decays, for instance, and was postulated by Wolfgang Pauli in 1930 to make up for losses in energy and momentum when atoms undergo beta decay (e.g. for a neutron to decay into a proton, it will emit an electron and a neutrino). Another fun neutrino fact is that 1 billion of them have probably passed through you as you finish this paragraph, mostly coming from nuclear interactions in the sun.

These four particles complete the **first generation**: e^- , d , u , and ν_e . As the name implies, there are additional generations – exactly two more, in fact, which is a stringent requirement of the mathematics of quantum field theory (though experiment could easily refute this in future). These generations are analogous to the first, each with something electron-like, two quarks, and a neutrino, with the generations differing by mass (abd name) alone. The second generation contains the muon μ^- , the strange quark s , the charm quark c , and the muon neutrino ν_μ , while the third contains the tauon (or just tau) τ , the bottom quark b , the top quark t , and the tau neutrino ν_τ . The full spread of these particles is shown in Figure 1.1, including details on the charges and relative masses (assuming the electron mass $m_e = 0.511$ MeV was actually 1 kg). And no, we have no idea why the top quark is a Big Chungus³.

Particles carry an intrinsic angular momentum, known as **spin**. If you want a mental picture, this can be thought of to some degree as the particles literally spinning in place, but it’s of course more a property of the field than the particles themselves. The main thing to note about spin is that it’s quantized into half-integer amounts (e.g. $1/2$, 1 , $1+1/2$ etc.), and the sign indicates the direction of that spin. Importantly, particles with half-integer spin cannot occupy the same location, which is known as the Fermi exclusion principle. We can also define the notion of **handedness**: a (massless) particle is left-handed if its spin vector and momentum vector are pointing in the same direction, and right handed if they’re pointing opposite directions.

²Beyond sounding remarkably like instructions to navigate a maze, these compositions actually hide a secret in their notation: they actually refer to three *additional* quarks, where there is a pre-existing sea of quarks already there in the vacuum, continually coming in and out of existence. The void is not as lonely as one may imagine.

³Here, I invite those unfamiliar with this term to use Google (or, at the time of writing, ChatGPT is probably more appropriate)

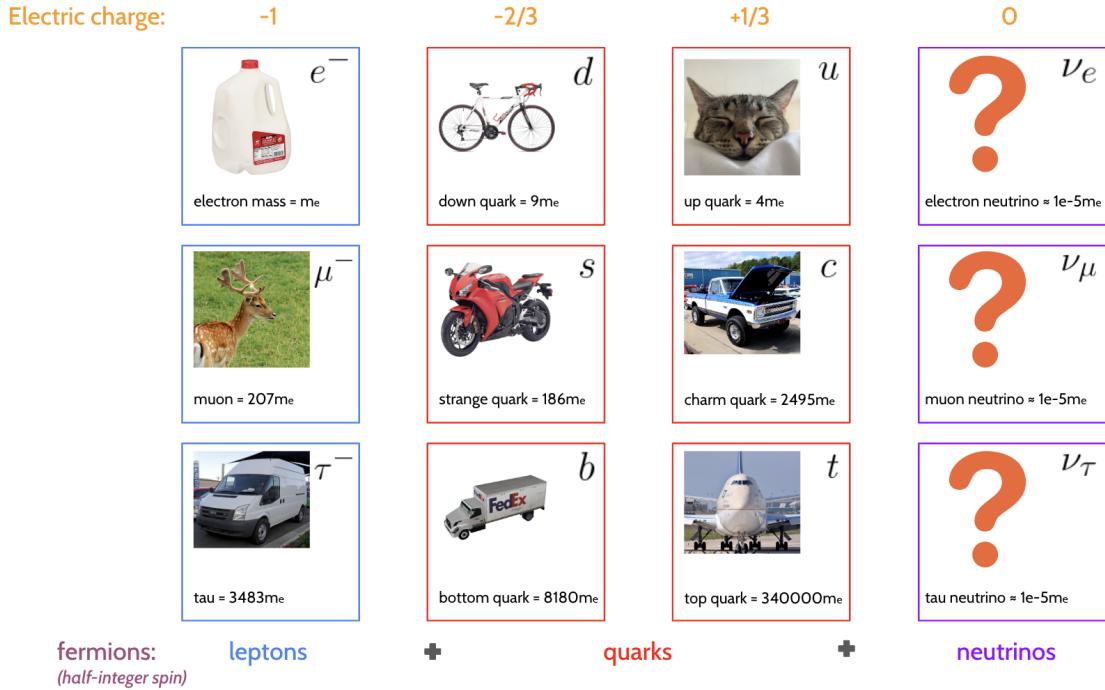


Figure 1.1: A cartoon schematic of the Standard Model fermions. Images are examples of objects that weigh about the same relative mass to the electron, assuming the electron weighed 1 kg.

We come to yet another notion of particles: **antimatter**. Each particle in the table above has an antimatter counterpart, denoted either with a bar over the letter for quarks and neutrinos ($\bar{u}, \bar{\nu}_\mu$) and through flipping the sign of the charge for leptons (such as the positron e^+). This is just notation; antimatter is a flipping of the sign of some of the basic properties of the particle, namely the electric charge and the handedness. We note here that whether the neutrino is its own antiparticle is a subject up for debate; it is unknown if right-handed neutrinos (or left-handed antineutrinos) exist at all.

1.0.1 Forces

When two particles feel a force, it's often said that those particles undergo the exchange of the relevant particle to that force, i.e. there's a *mediator* for every force in the form of a particle. But in my mind, this leads to weird images of some particles throwing other particles off one another, which is then somehow meant to manifest as something like gravity or magnetic attraction, neither of which seem intuitive⁴. Nevertheless, it remains a useful construct to think about these mediator particles from the perspective of the underlying mathematics. These particles that mediate forces carry integer spin, and are called **bosons** for this reason. Here are the main examples:

- The **electromagnetic force** (or hypercharge), carried by the **photon** γ
- The **weak force**, carried by three particles: the W^+ , W^- , and Z^0 bosons
- The **strong force**, carried by the **gluon** g (named for being the glue that keeps protons together)
- **Gravity**, which is not described by the Standard Model. In theory, one could have a force-carrying particle called the *graviton*, but this has no experimental evidence yet.

The Higgs field

To top off our description of the Standard Model, we mention the **Higgs field**, with a quantum of energy known as the **Higgs boson**. The field (and particle) are the only ones in the Standard Model without any spin, which is what we call a **scalar field**. This property leads to a surprising fact: the value of the Higgs field can be *non-zero in the vacuum*. The reason for this is due to the shape of the **potential energy** of the Higgs field, which can be loosely thought of as how much energy the Higgs field needs to have to take on a certain value. In the Standard Model, this potential $V(\phi)$, where ϕ is the value of the Higgs field, has the relatively simple form

⁴I would love to give an analogy here like waves getting bigger or smaller after exchanging different waves between them (since forces and particles are all excitations of fields), but I don't have enough grounding in the details to assert if it's a good one. Indeed, the “intuition” of a field theory is more just working through the large number of equations that describe an interaction, and then being content enough with your effort that you claim to have understanding of how it works. Instead of going down this rabbit hole, we'll take the scope-driven decision to leave a good reference and move on (e.g. [David Tong's QFT lecture notes](#)).

$$V(\phi) = a|\phi|^2 + b|\phi|^4 . \quad (1.1)$$

The Standard Model predicts the shape of this potential as shown in Figure 1.2, which is only possible with $a < 0$ and $b > 0$. In the absence of anything else, i.e. in the vacuum, the Higgs field will sit somewhere at the minima of this potential. But as shown in Figure 1.2, the values of the field in this valley are non-zero.

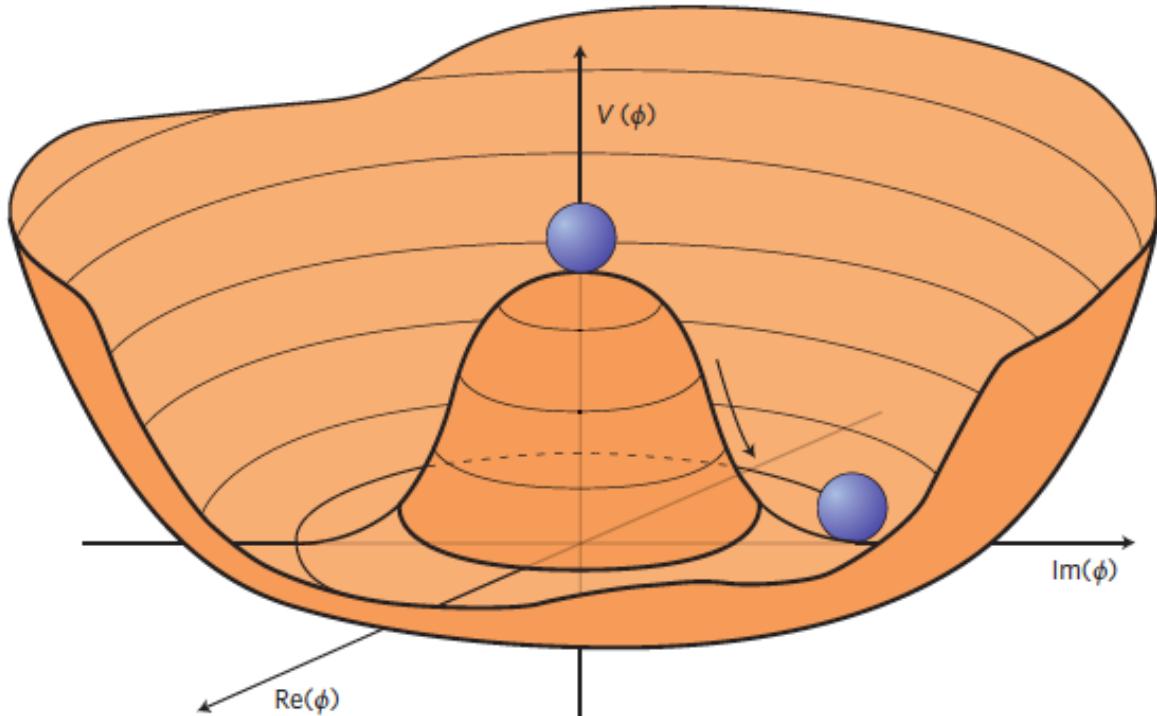


Figure 1.2: An example of the shape of the Higgs potential predicted by the Standard Model. A cartoon ball is shown to indicate that the Higgs will settle in one of the low-energy states away from the origin. Attribution: (Oxford University 2021)

A consequence of the Higgs field being “turned on” in the vacuum with some value of energy is that it is responsible for giving *fundamental particles mass*. Here, I stress the word “fundamental” – the mass of composite particles made of quarks (or **hadrons**) is actually due to large fluctuations of the associated quantum fields, where the Higgs-given masses are a negligible contribution (the mass of the proton is about $1836m_e$, which is clearly larger than two up quarks and one down quark from Figure 1.1). An often-quoted analogy that holds very delicately is treating the Higgs field as a thick, viscous liquid (think Marmite), and particles then gain mass as they move through it, with the amount of resistance depending somehow on the type of particle. This interaction is technically a fifth force called the Higgs force, but it’s not often quoted as such.

The particle discovered by the ATLAS and CMS experiments at CERN in 2012 is widely believed to represent the Higgs boson as proposed by the Standard Model (ATLAS-Collaboration 2012). This is largely due to the mass measured for the Higgs boson being consistent with the Standard Model prediction of $m_H \approx 125$ GeV. For something fairly up-to-date, a summary of Higgs mass measurements can be found in Figure 1.3. However, it is precisely the fact that the Higgs is this mass that has left the field of particle physics in a bit of a muddle. We'll touch on this at the end of the chapter.

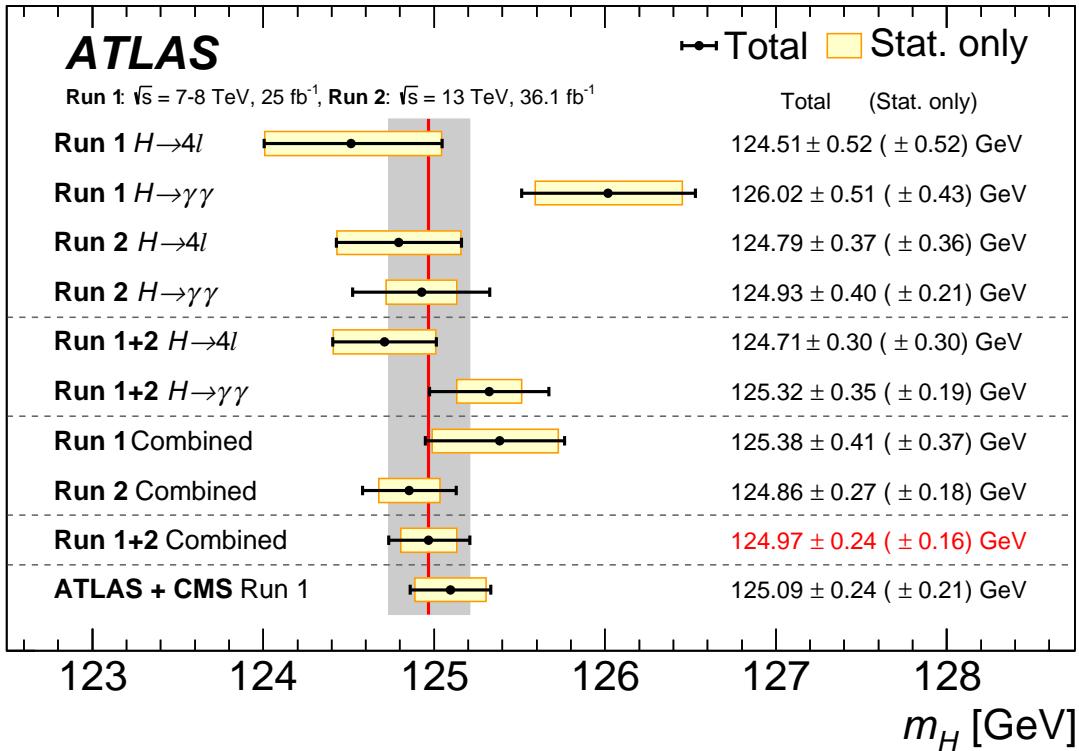


Figure 1.3: Summary of the main Higgs boson mass measurements with their associated errors.
Attribution: (ATLAS Collaboration 2022a)

Decays of the Higgs boson

For all this talk of the Higgs boson, it doesn't stop around for long. It has a lifetime of 1.6×10^{-22} seconds, which is a number smaller than a second by a factor of around a billion squared. The result of this is that the Higgs will decay into other particles nearly instantly within our particle detectors – we're then left to chase its shadow. The Higgs can decay into many different particle types, provided, of course, their total mass does not exceed that of the

Higgs (conservation of energy). However, it is more likely to decay to some things than others. These different probabilities for particles to decay into each variety are known as **branching ratios**, with the Higgs' most common decay being to two b -quarks. We can see these branching ratios as a function of the Higgs mass in Figure 1.4, where we have a little look either side of the measured mass from our experiments.

A general note on decays: you'll see decays to two quarks written sometimes as qq , bb etc, but any decay to two identical quarks means one of them is an anti-quark, for reasons of conservation of charge amongst other things. So $H \rightarrow bb$ means $H \rightarrow b\bar{b}$, just in case I'm not explicit in future.

1.1 Properties of particles (and their colliders)

Due to the equivalence of mass and energy (think $E = mc^2$), one could imagine the ability to create things with large mass, if we had enough energy to do so. That is precisely the idea behind **particle colliders**: we give particles a large amount of energy (i.e. they're traveling close to the speed of light), and then collide them so that they interact. These interactions, with sufficient energy, can then lead to the creation of heavier particles, provided that particle has mass that's less than the energy at which the particles that produced it collided. We call this energy the **center-of-mass energy**, which is around 13.6 TeV for run 3 of the Large Hadron Collider. This process of collision is usually done through charged particles such as protons, because we can accelerate them using electric and magnetic fields to speeds that can produce energies like this.

How do we detect if we produced the particles we want? We can do this by analyzing data from the collision; for that, we need to surround areas of our collider with **detectors**, which collect all the by-products that splash out from the center of the collision. These detectors, along with some input from software, have the ability to *reconstruct* the tracks that (charged) particles leave in the detector, from which one can determine properties like the charge from the way the track curves. Additionally, there are modules that can measure the energy deposited from particles emerging from the collisions, which can be placed at different distances to measure particles with different lifetimes (short-lived particles that decay quickly won't ever make it past a certain distance before being totally absorbed by the detector itself).

Given this, we'll go over some of the properties that particles have while moving, and why they're useful for looking at the validity of physical theories.

From here, we will use the convention of **natural units**, which essentially absorbs constant factors of the speed of light c and the Planck constant \hbar into the units chosen. You will then see quantities quoted in **electron volts** (eV) with different prefactors as usual for the size ($\text{GeV} = \text{giga electron volts} = 1 \times 10^9 \text{ eV}$ etc.). 1 eV is a very small amount of energy indeed (1.6×10^{-19} Joules), with the center-of-mass energy of the Large Hadron Collider being 13.6

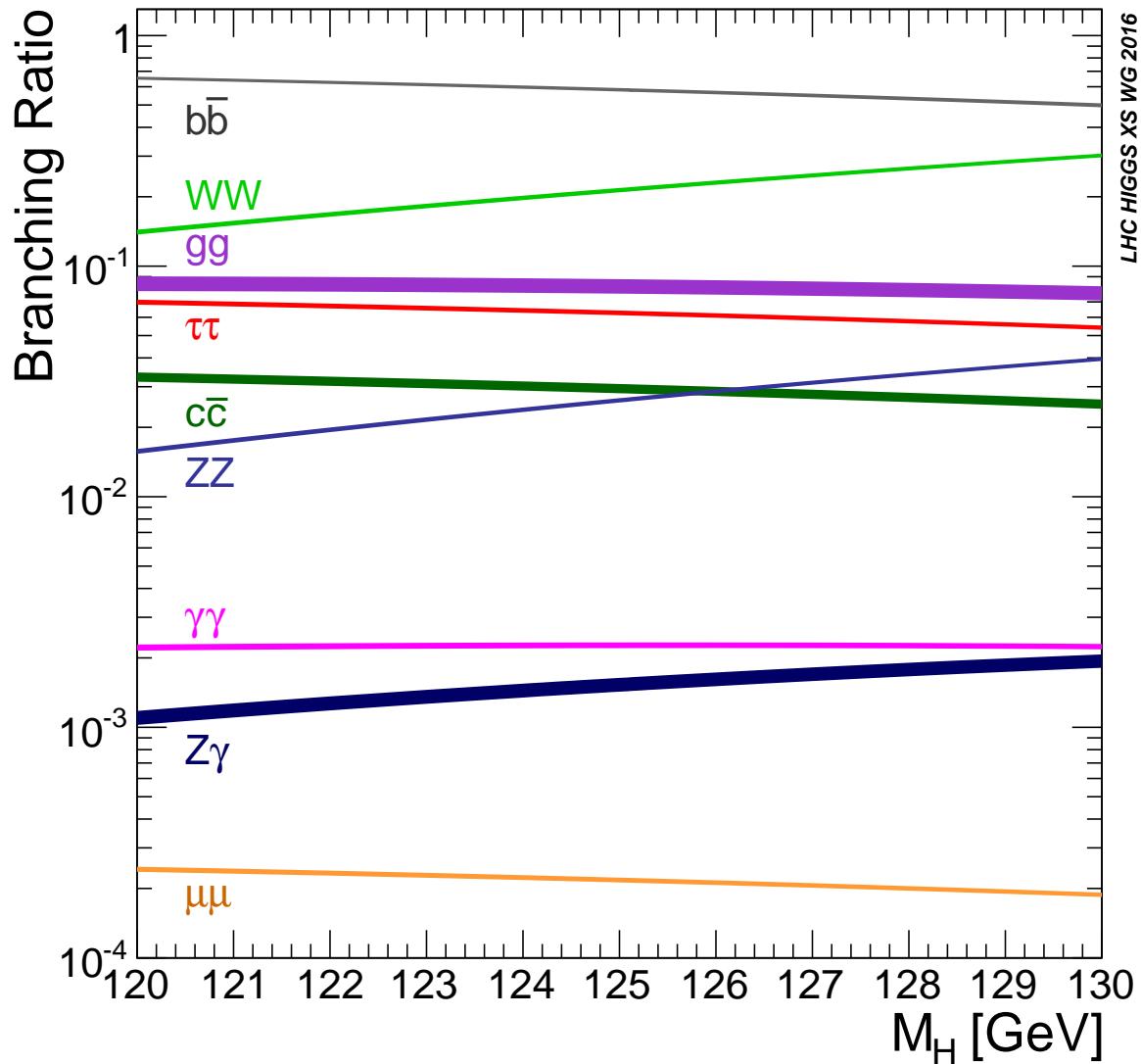


Figure 1.4: Branching ratios of the Standard Model Higgs boson to its main decay modes as a function of mass. Attribution: (CERN 2017)

TeV – still much less than a sandwich (but I would support building a sandwich collider; see (Doglioni et al. 2019) for an attempt of this nature, though physics results may vary).

1.1.1 Kinematics

We start with **relativistic kinematics**, i.e. how things move when they’re nearly at the speed of light. Objects like this are best described by talking about **spacetime**, which imparts an extra temporal dimension to the traditional three-vector for position in the form of a four-vector:

$$x^\mu = (t, x, y, z) = (x_0, x_1, x_2, x_3) .$$

Equivalently, we can drop the index μ from upper to lower, and get the equivalent $x_\mu = (t, -x, -y, -z) = (x_0, -x_1, -x_2, -x_3)$ (choice of convention). This allows for the compact notation of dot products between four-vectors using summation notation:

$$x^\mu y_\mu = y_\mu x^\mu = x_0 y_0 - [x_1 y_1 + x_2 y_2 + x_3 y_3] . \quad (1.2)$$

This quantity is important, as it can be shown to be *Lorentz-invariant*, which means the value remains the same even if we change the reference frame we’re in (i.e. we move in some way relative to the object). Using the four-vector for position, we can define a four-momentum:

$$p^\mu = m \frac{dx^\mu}{d\tau} ,$$

where m is the object **rest mass**, and τ is the **proper time**, defined by applying the relativistic factor γ to time as

$$t = \gamma \tau; \quad \gamma = \frac{1}{\sqrt{1 - v^2}}$$

for magnitude of the object’s three-velocity $v = |\mathbf{v}|$. This leads to an equivalent notation of

$$p^\mu = (E, \mathbf{p}); \quad E = \gamma m, \quad \mathbf{p} = \gamma m \mathbf{v} .$$

Using Equation 1.2, we can take the dot product of p^μ with itself:

$$p^2 = p^\mu p_\mu = E^2 - |\mathbf{p}|^2 . \quad (1.3)$$

We can exploit the fact that p^2 is invariant to its reference frame and examine one case in particular: a stationary body with 0 velocity but some mass will have a non-zero four-momentum $p^\mu = (m, 0)$. Then, we have $p^2 = m^2$, which we can set equal to Equation 1.3 that holds generally:

$$\Rightarrow E^2 - |\mathbf{p}|^2 = m^2 , \quad (1.4)$$

which is called the **energy-momentum relation**, and leads to the left-hand side being known as the **invariant mass** s , since it recovers the rest mass of a body in that body's rest frame. Of course, \sqrt{s} is then the actual rest mass in this case, which is why we write $\sqrt{s} = 13.6\text{ TeV}$ as the center-of-mass energy for the LHC.

For multiple particles, Equation 1.4 then gives rise to the concept of the invariant mass of a system of bodies with four-momenta p_1, p_2, \dots – their total momenta is $\sum_i p_i$, and the total invariant mass is then

$$s_{1,2,\dots} = \left(\sum_i p_i \right)^2 , \quad (1.5)$$

which will involve terms in the energies and three-momenta of the different particles as per Equation 1.4. This quantity will be particularly important when we come to the search for a new particle in the latter stages of the thesis, because it allows us to detect **resonances**, which are intermediate particles that can produce a different final state. As an example, the Higgs boson can decay to four leptons via other vector bosons as per Figure 1.4 (e.g. two Z bosons can each decay into two leptons), meaning the Higgs can then be found in the invariant mass of this four-lepton system, m_{4l} . We can see this in Figure 1.5, where there's a peak at the Higgs mass of $m_H \approx 125\text{ GeV}$, since the invariant mass of the initial state (a Higgs boson with $E^2 - |\mathbf{p}|^2 = m_H^2$) is equal to that of the final state (four leptons) by energy/momentum conservation.

1.1.2 Quantifying collisions

An interaction between colliding particles (that usually produce some measurable detector output) is called a **scattering event**, or more simply just an **event**. To cause an event then, indeed, particles must collide. What's the chances of that happening? If we were instead talking about two tennis balls colliding, there would be an idea of a cross-sectional area influencing this, whereby if the tennis ball were to enter that region, collision of some variety would occur due to the balls being close enough, with the rate of this occurring being related to the size of that area. A similar quantity exists for particles colliding, which we call the **scattering cross-section σ** (or just cross-section). The details on how one calculates a cross-section are more complicated for particles, but quantum field theory has exact rules for this that involve quantities called

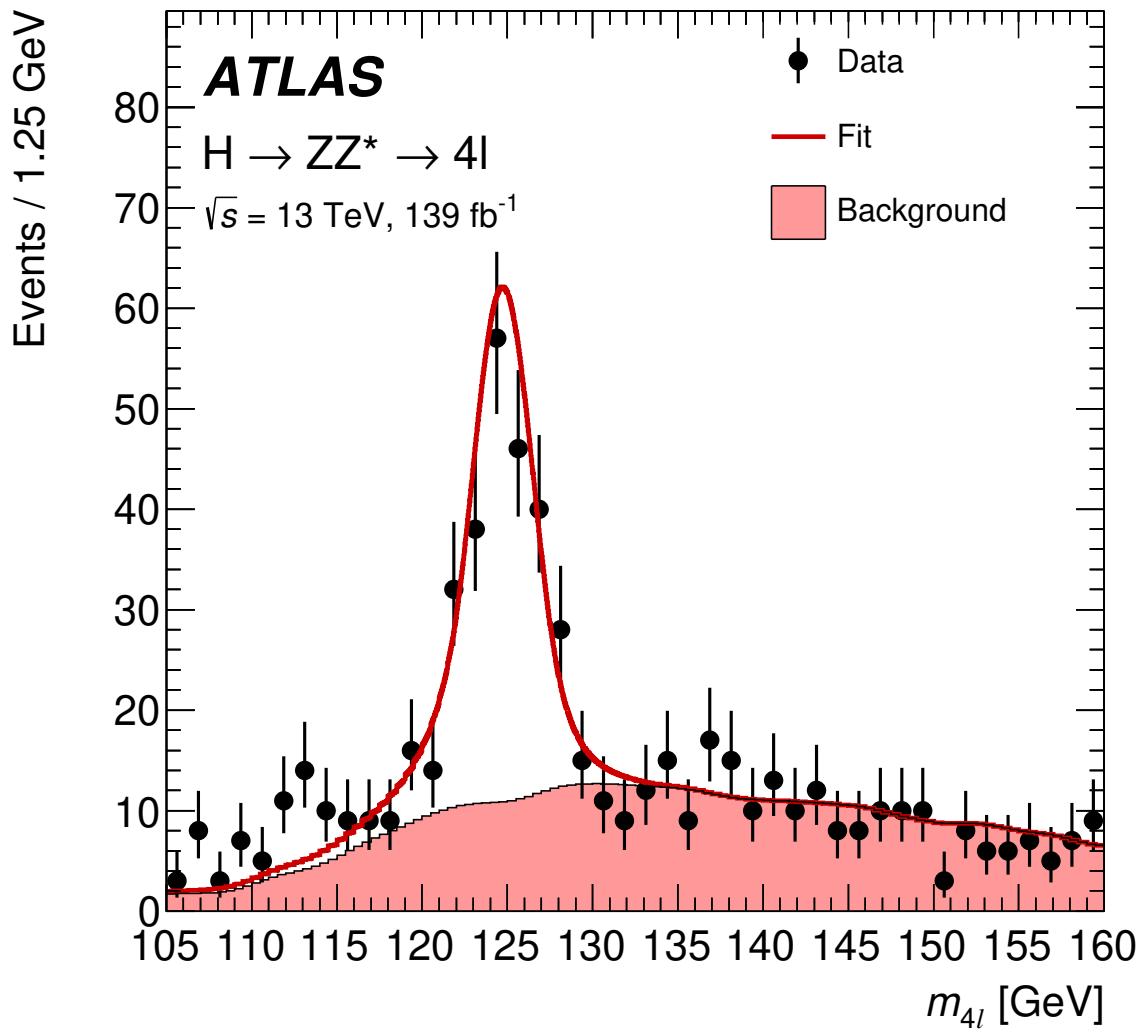


Figure 1.5: An example plot of the four-lepton invariant mass, taken from a recent Higgs boson mass measurement in this final state. Attribution: (ATLAS Collaboration 2022b)

scattering amplitudes, and also performing an integral over the space of momenta of the initial state particles. I omit the details as they are beyond the scope of my work – see e.g. section 2.7 of (Buckley, White, and White 2021) for more. We will go as far to state this: given a number of scattering events N (every interaction between some set of colliding particles), the rate of these events occurring is directly proportional to the cross-section, i.e.

$$\frac{dN}{dt} \propto \sigma \quad \Rightarrow \quad \frac{dN}{dt} = \mathcal{L}(t)\sigma , \quad (1.6)$$

where we've denoted the constant of proportionality as the **luminosity** $\mathcal{L}(t)$, which generally can be a function of anything to do with the structure of the colliding objects (e.g. beams of particles) at some time t . We can see that increasing $\mathcal{L}(t)$ increases the event rate; this leads to the analogy of beams of colliding particles being “brighter” with higher luminosity, hence the name.

We can also state that the overall cross-section of some collision is equal to the sum over the cross-sections for mutually exclusive physics processes i (as to not double count): $\sigma = \sum_i \sigma_i$, and we have individual equations

$$\frac{dN_i}{dt} = \mathcal{L}(t)\sigma_i .$$

The take-home from this is that for any physics process, the event rate in a collision will be a function of a term that dictates the underlying physics (σ_i) and a term that is influenced by beam structure ($\mathcal{L}(t)$). Moreover, we can define an overall **integrated luminosity** L as a metric of cumulative beam “brightness” up to some time T by integrating Equation 1.6:

$$L = \int_0^T \mathcal{L}(t)dt = N/\sigma .$$

The cross-section has units of area (m^2), and is usually quoted in *barns*, where $1 \text{ b} = 10^{-28} \text{ m}^2$. Since N is unitless, the luminosity then has units of inverse barns, which are usually quoted at the femto scale (fb^{-1}).

1.2 Particle detectors

We'll say a few words on the detectors that are used to measure these particle collisions, with a focus on the ATLAS detector at CERN ATLAS Collaboration (2008).

ATLAS is the name for both the detector that wraps around part of the beam pipe at the Large Hadron Collider, the experiment that it conducts, and for the collaboration of people that work on building the detector and analyzing the resulting data. The detector itself is split

up into four concentric parts: the **inner tracking detector**, **electromagnetic calorimeter**, **hadronic calorimeter**, and the **muon detector**, which are in the toy schematic shown in Figure 1.6. Each part has a different job, which is summarized in the following paragraphs.

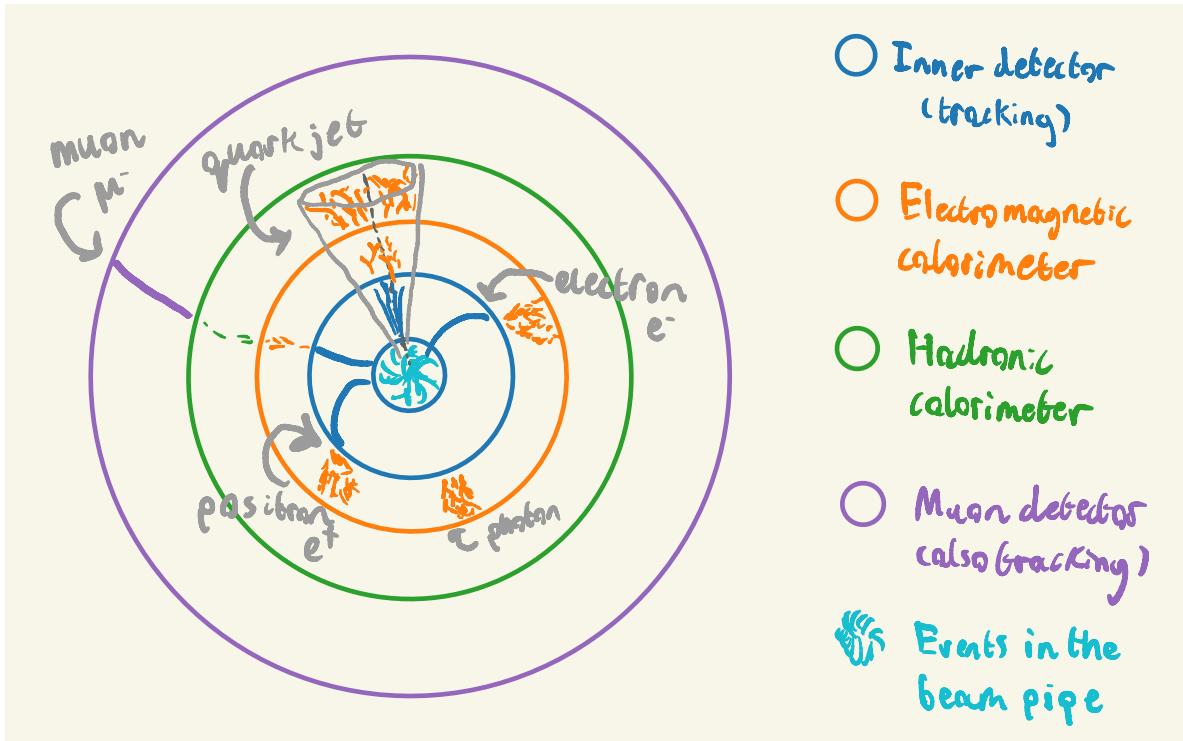


Figure 1.6: A toy schematic for the transverse cross-section of an imagined particle detector for collisions of two beams. The signatures different types of particles would leave are depicted within the detector.

The inner detector tracks charged particles that leave *hits*; these come from things like ionization of a gas as the particle moves through, and having charged wires that collect the free electrons from the ionization. By trying to intelligently draw a line through these hits, e.g. by fitting a functional form, we can reconstruct the shape of the track. To measure the properties of charged particles emerging from collisions like the charge and momentum, we can look at the curvature of the track. To bend particles in the detector so that they have curvature, we need to apply a magnetic field that causes the particles to move in circular motion in the transverse plane (i.e. perpendicular to the direction of the beam). ATLAS does this by surrounding its inner detector with a solenoid magnet (and toroidal magnets on the barrel and endcaps).

You'll have noticed there are two calorimeters – this is because electrons and photons penetrate material much less deep than hadrons, so they're separated into two different parts. Calorimeters in general measure *energy deposits* by having the particles collide with some dense material, which causes energy loss in some way, and then interlacing that material with something that

can collect information on the energy of the resulting products from traveling through the dense medium. The *electromagnetic calorimeter* is responsible for doing this for electrons and photons, where they undergo energy loss by scattering and Bremsstrahlung radiation. It's worth noting that quarks are never observed standalone in a detector. Instead, they rapidly decay into sprays of collimated **hadrons** (particles containing quarks) by the process of hadronization. We refer to these structures as particle **jets**. The *hadronic calorimeter* exists to detect hadrons from these particle jets, where their main source of energy loss is scattering processes with the calorimeter material.

The final part is the muon detector, which sits external to all other detectors, and is also a tracking detector like the inner detector. The muon passes through the inner detector and calorimeters, but typically will not lose much energy like other particles might from scattering or Bremsstrahlung. That means that if we have a tracking detector far from the beam pipe, it's likely that anything it picks up will be a muon.

1.2.1 Kinematics, again

Using the information the detectors give us, we can summarize an event by the properties of the objects that the detector picked up as a result. We can think of an event as a list of particles with four-momenta, and one additional entry that has the missing four-momentum compared to the total initial proton four-momenta, which could include particles invisible to the detector like neutrinos. These four-momenta are typically transformed to a different set of coordinates that better fit with describing the geometry of the detector itself.

If we denote the beam axis as the z direction, the x - y plane is known as the **transverse plane**, which groups the three-momentum of a particle into $\mathbf{p} = (\mathbf{p}_T, p_z)$. One will often hear about the magnitude $p_T = |\mathbf{p}_T|$ being a quantity of interest, which is due to the fact that objects with high p_T will likely be much easier to reconstruct and measure precisely, since they are not mixed up with all of the colliding proton beam debris in the z -direction. For this reason, we're actually not able to measure p_z very well, and instead look to variables that are *invariant* to changes in velocity in the z direction. One example of a quantity like this is the **rapidity**, defined as

$$y = \frac{1}{2} \ln \left(\frac{E + p_z}{E - p_z} \right),$$

which measures how “forward” (close to the +ve z axis) or “backward” (close to the -ve z axis) a particle lies. $y = 0$ corresponds to no z component of the momentum, and $\pm\infty$ means the momentum is aligned with the +ve and -ve z direction respectively. Particle physicists often use the **pseudorapidity**, defined as

$$\eta = -\ln \left(\tan \frac{\theta}{2} \right),$$

which is equal to the rapidity for particles with energy E much higher than their mass m . It's preferred since the polar angle θ between z and the transverse plane is much easier to determine than p_z , for instance. We can thus fully specify a particle's position in the detector with the (pseudo)rapidity and the azimuthal angle ϕ between the x and y directions.

1.3 Simulators

We are not able to perform our data analysis on collisions where we *know for sure* what produced them. If we could access this information, that would allow us to do many practice runs where we tune things to give us the best chance to discover the signal, if it was actually there. To this end, countless generations of particle physicists have worked on building robust **simulators** that can produce many Monte Carlo events (read: randomly sampled events from physics distributions). They work by calculating the different terms in an expansion as set out by quantum field theory responsible for the rates of physics processes, known as *perturbative field theory*, to a specified order in the expansion. This is what is referred to by phrases like *leading order* (LO) and next-to-leading order (NLO) – it's the choice of terms you include in the perturbation calculation, which corresponds to choosing to include the different ways to produce that given final state you want to produce.

After simulating the physics processes themselves, we're not quite ready to jump in and optimize our analysis code, because we're not looking at something that mirrors what we'd expect from our detector. As an example, it's likely that our detector is only able to measure particle momenta up to a certain *resolution*, but we have access to the true values with no uncertainty. To change this, we can apply a layer of functions that attempt to *smear* the output, e.g. by sampling momentum from a normal distribution centered around the true value instead of using the true value directly, which should mimic the fact that we're inherently limited in the way we can measure these quantities in real life. Moreover, we won't be encountering the values of momentum – we'll be getting electrical signals from a wire! We need to then do the additional step of **digitization**, which turns the physics quantities into things we'd expect from a detector, such as track hits and energy deposits.

Once we've done all that, we're free to then attempt to **reconstruct** the events just like we would for a regular detector (essentially building up particle four-momenta from track information), which allows us to make sure we don't do any better in getting the physics information than we would be able to in actuality. We can then use this information as the input for our physics analysis, and begin to optimize. The only difference is that there's a bias between the simulation and real data we may struggle to account for, but we trade off by having a label on each event that tells us which physics process it came from (i.e. signal or background). We can see this whole process depicted in Figure 1.7.

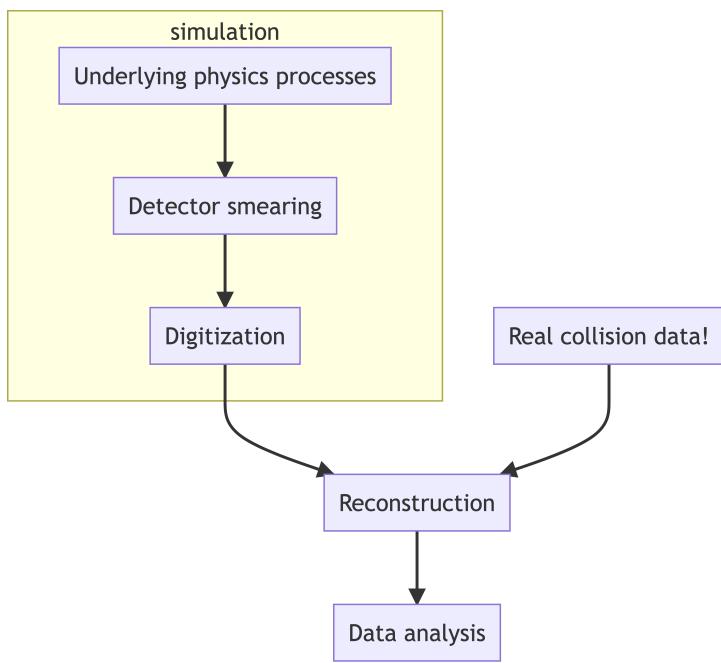


Figure 1.7: A summary of the different workflow steps that are taken when simulating particle physics processes, including mirroring detector effects.

1.4 Issues with the Standard Model, and what may lie beyond

Here we touch on a few of the cracks in the Standard Model, and some proposed resolutions. We'll only explore enough to get an idea that it's certainly worth searching for these solutions in some way!

1.4.1 The hierarchy “problem”

A property unique to the Higgs boson is that its measured mass is very sensitive to physics at higher energy scales (read: new particles with higher masses than discussed here), so the fact that the Higgs is fairly light at 125 GeV is a strong constraint on the scale of new physics that we're likely to see. Let's explore a little why this is.

Now, in a bit of an aside, quantum field theories are able to work well due to a process called **renormalization**, which essentially amounts to subtracting away infinite quantities that can arise in calculations involving fields. A consequence of this is that all parameters of a quantum field theory are inherently linked to some energy scale (or equivalently distance scale) at which we admit our ignorance, i.e. there's an energy *cutoff* at which we say our theory no longer applies at energies higher than this. We term that cutoff Λ_{UV} . One surprising thing about the choice of Λ_{UV} is that it actually impacts the value of the Higgs mass! This is because similar to hadrons, the Higgs boson gains its own mass in part due to the quantum fluctuations of many different fields, with Λ_{UV} controlling the scale of these fluctuations. These are colloquially termed as quantum “corrections” to the value of the mass. So when we measure m_H , what's actually beneath the curtain? It turns out that m_H is then actually made up of two parts:

$$m_H^2 \approx |a + \mathcal{O}(\Lambda_{\text{UV}}^2)| \approx 125 \text{ GeV} ,$$

where the parameter a is part of the formula for the Higgs potential in Equation 1.1. This a parameter, which is usually referred to as the *bare mass* (i.e. what would be the mass in the absence of corrections), is that it has to be large and negative if Λ_{UV} is of any reasonable size in order to cancel out their values enough to get 125 GeV.

This isn't necessarily a problem, per se, but it's quite the coincidence if true. To be as kind as possible to us, we can say Standard Model is no longer valid just above the current energy scale of the LHC (13600 GeV), which would make the parameter a be of a similar size such that their sum results in 125 GeV. This would mean we'd see some new theory come into play around the TeV scale, which we haven't found evidence for. Of course, to see *pretty much no signs* that there's new physics at this energy scale, we'd probably hedge our bets that it holds a bit further out than this, which would lead to numbers much larger (hundreds of thousands) having to cancel out precisely to 125 GeV. Again, this isn't necessarily an issue – nature could just be very fine-tuned. But this is a source of unease for many theoretical physicists, and it remains an open “problem” to find out why this is the case.

1.4.2 Gravity

It is unfortunate that such a well-tested theory does not adequately describe gravity, which, at the time of writing, seems to still be doing its thing. Moreover, Einstein's theory of General Relativity, which describes gravity, doesn't seem to fit well with all this particle talk, but it too is a very well-tested theory. This is one of many frustrating things about having the Standard Model triumph experimentally: we *know* it's not good enough alone⁵, and it somehow has to interplay with another very important theory, despite these puzzle pieces having wildly serrated edges. So yeah, we're not too happy about this.

1.4.3 Other things

More problems we don't have an answer to include:

- Why do we live in a matter dominated universe instead of antimatter?
- Do the forces of nature unify at a certain energy scale?
- What's the deal with dark matter?
- ...and many more!

All of these questions have potential answers involving both new physics theories and verifiable experimental consequences (which makes them well-posed theories). The agenda of the LHC and many other particle physics experiments is then to probe them however we can, with the tools available to us.

1.4.4 Going beyond the Standard Model

Just to mention one, the most commonly touted theory that has been investigated in recent years is *supersymmetry*, which makes it such that every particle proposed in Figure 1.1 has a supersymmetric partner at some higher energy scale⁶. Importantly, these additions help to stabilize the mass of the Higgs boson in the hierarchy problem, and also conveniently helps with unification of forces. It's actually all quite neat, but has the large drawback of a total lack of evidence for its existence.

There are many more theories of this nature, including many exotic new particles and ideas, but none seem to have poked their head out at any of our experiments as of yet. That's why it remains paramount to both look for these new hypothesized particles and also precisely measure things that the Standard Model predicts, which may act as a calling card for a new theory we have yet to discover.

⁵I've heard water cooler talk about particle physicists even being upset at the Higgs discovery for this very reason – a nail in the coffin for many other theories.

⁶These particles have super cute names like sleptons, squarks, gluinos... I highly recommend reading the Wikipedia page.

2 Probability and Statistics, in theory

It must be said that I have no desire to subject you, the reader, to the same philosophical torment that I have undergone in my pursuit of clarity of this topic, which I could not even claim to have reached. Moreover, given that this is an *experimental* physics thesis, it is exceedingly likely that you are a pragmatist, and wish to move swiftly on to the sections that may be useful to your life. Nonetheless, I'd like you to allow me the courtesy of proposing that there may in fact be something truly useful in revisiting these foundations, if only to reaffirm their non-utility.

For this section, my most heavily used and recommended resource is (Cousins 2018), which I heard Bob himself refer to as his “life’s work”. Do give it a read – so many useful gems by someone who took a lot of time to build bridges between science and statistics!

2.1 Probability, distributions, and likelihood

Both the pre-amble to and the beginning of my PhD studies were decorated with thoughts on the nature of probability. At the time, I had just come out of a Masters degree project that involved the application of *nested sampling* Skilling (2006) to infer the momenta of invisible neutrinos. This technique was invented by John Skilling, a prolific figure in the realm of Bayesian statistics, if only for his advocacy thereof (if you’re planning to be indisposed for a time, you may find Skilling (2008) of interest as reading material, but do make sure to dilute it with things like Senn (2011) and Mayo (2018)). This started me down a rabbit hole on the much-contended topic of the definition of probability. It turned out the topic was vast, with arguments both mathematical and philosophical dating back many hundreds of years, many of which are still alive in the present day. Of this, I was particularly surprised — my undergraduate courses had spent a mere ten minutes or so on the subject, and I thought I understood it perfectly well given the time allocated! “Surely”, I mused in confusion, “probability, as I’ve encountered it both intuitively and mathematically, is just

$$P(A) = \frac{\text{number of occurrences of } A}{\text{total number of occurrences}} , \quad (2.1)$$

right?”

Alas, the contentious nature of humanity would not allow me such a privilege. However, it is from this place of existential angst that we shall proceed, and uncover where this definition of probability encounters its limits (but also where it is useful).

2.1.1 Axioms of probability theory

For probability P (whatever you think it means), and possible states of an event Ω , we can say for $A \in \Omega$:

- $P(A) \geq 0$ always
- $P(\Omega) = 1$ (at least *one* event will occur)
- The union (\cup) of variables $P(A \cup B \cup C) = P(A) + P(B) + P(C)$ for *mutually exclusive* events $A, B, C \in \Omega$ (i.e. only if they cannot occur at the same time)

The next notion to cover is that of **conditional probability**:

$$P(A \cap B) = P(A|B)P(B) . \quad (2.2)$$

Depending on whose axioms you follow, this quantity may be either derived (as in (Shafer and Vovk 2006)) or axiomatically stated (as in (Finetti 1970)). We can also expand this definition generally to include as many variables as we want, e.g. for 3 variables:

$$P(A \cap B \cap C) = P(A \cap C|B)P(B) = P(A|C, B)P(C|B)P(B) ,$$

and then for N variables:

$$\begin{aligned} P(\bigcap_{i=1}^N X_i) &= P(X_1|X_2, \dots, X_N)P(X_2|X_3, \dots, X_N) \dots P(X_{N-1}|X_N)P(X_N) \\ &\Rightarrow = \prod_{i=1}^N P(X_i|X_{j>i}) , \end{aligned} \quad (2.3)$$

where $X_{j>i}$ represents the set of all X_j for which $j > i$. This is known as the **probability chain rule**.

The axioms above lead to several other properties. For instance, the notion of conditional probability leads to the equation known as Bayes' Theorem:

$$\begin{aligned} P(A \cap B) &= \frac{P(A|B)}{P(B)} ; \quad P(B \cap A) = \frac{P(B|A)}{P(A)} \\ \Rightarrow P(A|B)P(B) &= P(B|A)P(A) , \end{aligned} \quad (2.4)$$

since the notion of “and” (\cap) is not position-dependent, i.e. $P(A \cap B) = P(B \cap A)$. This equation allows for the inversion of conditional probability, as long as we can provide the individual probabilities for A and B . For example, the age-old situation of $P(\text{positive test}|\text{have disease})$ versus $P(\text{have disease}|\text{positive test})$. See (Cousins 2018) (and countless other introductions to probability) for a worked example along these lines.

Another important notion is that of **independence**:

- For *independent* events A, B , $P(A|B) = P(A)$ (i.e. their venn diagrams don’t overlap, so the occurrence of B cannot influence A)
 - This also implies $P(A \cap B) = P(A)P(B)$

Independence is an important assumption for HEP – we assume that events in our particle colliders occur without influencing each other. This assumption fundamentally changes any modelling we do of a collider physics process in a probabilistic sense, as it reduces the modelling to event-level probabilities (and the joint distribution over all events is recovered through multiplication as above).

2.1.2 Interpretations of P

The previous section discussed axioms and properties for probability P that hold regardless of interpretation. However, when we start to give meaning to A, B, Ω etc, this can pose issues. For something like a coin flip, this isn’t too much of an issue – we can ask what the chances of observing the number of occurrences of $A = \text{heads}$ or $B = \text{tails}$ in some number of experiments N . This is known as the **frequentist** interpretation of P – literally the *frequency* of that possible outcome. But what if, for example, I let $A = \text{“The sky is blue right now”}$? Clearly it will be blue or it won’t be blue, so you’d imagine that perhaps the probability is $1/2$ if we use the definition of P in Equation 2.1. This isn’t particularly useful though – since I said *now*, there’s only one data point we could ever take, and that would be to look at the sky. There’s no way to take into account the fact that we may live in a very rainy city during winter, or if the sun exploded (I hope it didn’t do that yet).

The reason we faced issues there is because we tried to *assign a probability to a fact*. Similar questions could look like “what is the probability that the Higgs Boson exists?”, or “what are the odds of the next prime minister of the U.K. being a walrus?” – they’re all things that will either be true or untrue. We may like to make some probabilistic statements about these facts though (I’m particularly interested in the chances of the latter question): to do this, we need to shift our interpretation of P to a *personalistic degree of belief*. This is known as the **Bayesian** interpretation of probability.

Now, doing things the Bayesian way doesn’t mean we assign probabilities to facts with no reason (though we are free to do so). We end up incorporating **prior information** on these facts, e.g. the probability of it raining generally in your area, through Bayes’ theorem in Equation 2.4

($P(A)$ and $P(B)$ could play that role). Note, however, that Bayes' theorem stems from the axioms of probability, and *does not require Bayesian* P . It's unfortunate that Bayesian and Bayes' theorem are named as such, otherwise this would be clearer. Bayesian inference does, however, tend to use Bayes' theorem for conditional inversion. See Section 2.3.5 for more on this.

2.1.3 Probability density

We now shift our discussion from the big P to the small p , which is used to indicate the **probability density function** (pdf), defined implicitly through

$$P(a \leq X \leq b) = \int_a^b p_X(x') dx' .$$

Here, we're using capital letters for **random variables** (the thing that follows the distribution), and realizations of that random variable are in lowercase letters. We can also define the **cumulative density function** (cdf), defined for random variable X as $P(X \leq x)$. We can then write this in terms of the probability density function:

$$P(X \leq x) = \int_{-\infty}^x p(x') dx' .$$

This gives us the relation

$$p_X(x) = \frac{dP(X \leq x)}{dx} .$$

Pretty much all the same relations for big P also hold for small p , which can be attributed to many reasons (it's a rabbit hole involving measure theory and similar concepts – see Shafer and Vovk (2006) for more, it's well-written!)

2.1.3.1 i.i.d.

A common expression you'll see about a set of random variables is that they're **i.i.d.**, which stands for *independently and identically distributed*. This refers to the situation when

- Samples are drawn from the *same probability distribution*
- Each sample drawn (random variable) is independent from any other sample

An example is just drawing some random sample, e.g. `np.random.uniform(size=10)`. That would be 10 i.i.d. samples from a uniform distribution.

2.1.4 Change of variables formula

If the distribution over x is $p(x)$, what's the distribution over $\log(x)$? Or, more generally, any monotonic function $y = f(x)$ with corresponding random variable Y ? Let's look at the cdf:

$$P(Y \leq y) = P(f(X) \leq y) = P(X \leq f^{-1}(y)) .$$

Differentiating both sides with respect to y to recover the pdfs:

$$\frac{dP(Y \leq y)}{dy} = \frac{dP(X \leq f^{-1}(y))}{df^{-1}(y)} \frac{df^{-1}(y)}{dy} \Rightarrow p_Y(y) = p_X(f^{-1}(y)) \left| \frac{df^{-1}(y)}{dy} \right| ,$$

where we've inserted the absolute value to ensure this holds for both monotonically increasing and decreasing functions. The multi-dimensional version of this involves the determinant of the **Jacobian matrix**, defined for a function involving vectors $\mathbf{y} = f(\mathbf{x})$ as

$$J_f(\mathbf{x}) = f'(\mathbf{x}) = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix} . \quad (2.5)$$

This leads to the formula

$$p_Y(\mathbf{y}) = p_X(f^{-1}(\mathbf{y})) \left| \det J_{f^{-1}}(\mathbf{y}) \right| , \quad (2.6)$$

which can be thought of as manipulating the space in the x - y plane (since determinants are akin to volume transforms) to make the probabilities match. This will be particularly useful when we come to look at normalizing flows.

2.1.5 Expectation values

The expectation value for a quantity $f(x)$ over a distribution $p_X(x)$ is defined as

$$\mathbb{E}_{p_X}(f(x)) = \int_{-\infty}^{+\infty} f(x)p_X(x)dx ,$$

which I loosely think of as the average value that $f(x)$ will have assuming probability distribution p_X . Expectation values are useful to extract a definite value from a probability distribution, with many useful quantities such as the mean, variance, skew, and kurtosis all being able to be written in terms of expectation values (see more on this and the “moments” of a distribution in [this thoughtful blog post](#)).

2.1.6 Commonly used distributions

2.1.6.1 Normal

We define the **normal distribution** – commonly known as a “Gaussian” in HEP – with the pdf

$$p(x|\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}.$$

The parameters μ and σ characterize the location and the width of the normal distribution respectively. In shorthand, we’ll denote this as $\text{Normal}(\mu, \sigma)$, or maybe also including the input x via $\text{Normal}(x|\mu, \sigma)$.

The normal distribution is exceedingly useful as a modelling tool due to the *central limit theorem*, which states that the distribution of the sum (and consequently the mean) of i.i.d. random variables calculated on a sample tends to a normal distribution as the size of your sample goes to infinity. This type of distribution is known as a **sampling distribution** as it involves a quantity that is computed on a per-sample basis.

The specific normal distribution you end up with from the central limit theorem is $\text{Normal}(\bar{\mu}, \bar{\sigma}/\sqrt{n})$, where $\bar{\mu}$ and $\bar{\sigma}$ are the sample mean and standard deviation respectively. Part of the power of the central limit theorem is that it works regardless of the shape of the original distribution! So it’s pretty impressive that we can get a good idea of how the distribution of the data mean looks, even with a finite sample size.

2.1.6.2 Poisson

Another very common distribution in HEP is the **Poisson distribution**. It’s useful when you want to model the occurrence rate of an event (and what happens on average). It’s defined for *independent events* n as

$$p(n|\lambda) = \frac{\lambda^n e^{-\lambda}}{n!} ,$$

where λ is termed the *expected number of events* (both the mean and variance turn out to be λ). We’ll denote this using the shorthand of $\text{Poisson}(\lambda)$.

One commonly used notion is the approximation of a Poisson distribution with a normal distribution with mean λ and variance $\sqrt{\lambda}$ for large λ . We can see this demonstrated in Figure 2.1, where from $\lambda \approx 10$, we start to observe the alignment of the shapes of the Poisson and normal distributions. This is the origin of the \sqrt{n} errors that are often quoted on histogram bars of size n – it assumes they are Poisson modelled (as we do when modelling likelihood

functions in HEP), and if n is around 10 or more, then we assign \sqrt{n} as a notion of the standard deviation on the bin count n .

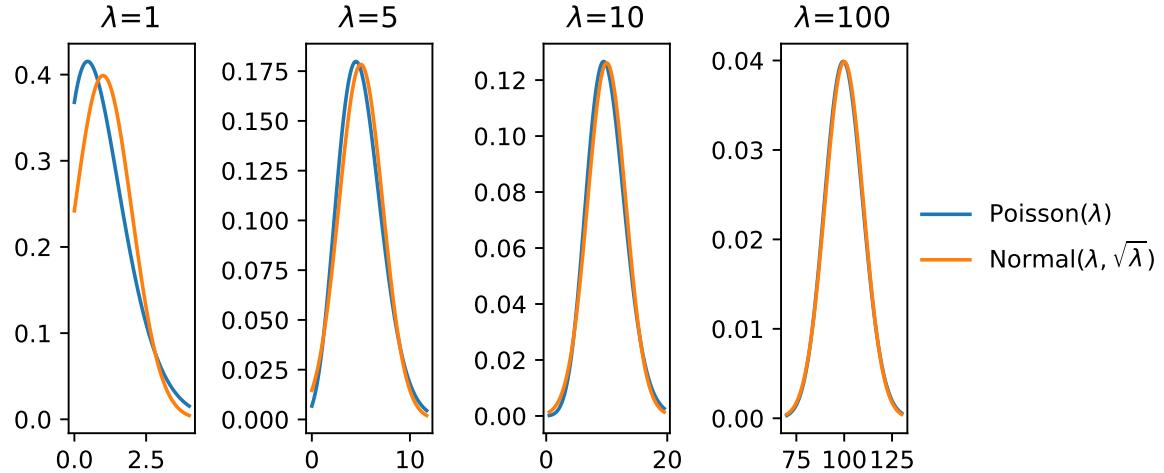


Figure 2.1: Comparison of the Poisson distribution at different values of λ with a normal distribution with mean λ and variance $\sqrt{\lambda}$.

2.1.6.3 Uniform

The **uniform** distribution is a very simple construct, with pdf

$$p(x|a, b) = \begin{cases} \frac{1}{b-a}, & \text{if } x \in [a, b] \\ 0, & \text{otherwise} \end{cases}.$$

We'll use the shorthand of $\text{Uniform}(a, b)$. When we refer to drawing values “at random”, we're probably referring to drawing $x \sim \text{Uniform}(0, 1)$.

2.1.7 Nuisance parameters

When our probability model $p(x|\mu)$ fails to describe the data generating process well, we may add more parameters to our model in order to make it more flexible, and thereby hopefully increase the accuracy of the model. As an example, this could be a parameter that controls the shape of the overall distribution in a way that models a physical effect. Such parameters are called **nuisance parameters**, as they exist only to add model flexibility (we're not interested in inferring their true values), and are then a nuisance to deal (increased dimensionality of any downstream calculations). If we denote the set of nuisance parameters of a model as θ , our likelihood then reads $p(x|\mu, \theta)$.

If we have some prior knowledge about θ , e.g. from a previous experiment that measured the physical event on data y (termed “auxillary data” since it isn’t directly to do with our main experiment), it would be useful to use that to constrain possible values θ could take. In a Bayesian setting, this prior knowledge can be added when defining the prior distribution for that parameter at inference time. It’s also possible to bake this information into the probability model itself through constructing the joint likelihood of both experiments:

$$p(x, y|\mu, \theta) = p(x|\mu, \theta)p(y|\theta) .$$

In the case where the distribution $p(y|\theta)$ isn’t readily available, it’s common practice in HEP to approximate it using a distribution that models the shape of the data y to some reasonable degree of accuracy, e.g. with a normal distribution of mean θ (this will be discussed more later).

To extract information about parameters of interest μ from a likelihood that involves θ , we need to somehow lose our dependence on θ to recover a distribution that just depends on μ . The ways of doing this are as follows:

Profiling: for each value of μ , find the best fit value of θ , leading to

$$p_{\text{profile}}(x|\mu) = p(x|\mu, \hat{\theta}); \quad \hat{\theta} = \underset{\theta}{\operatorname{argmax}}(p(x|\mu, \theta)) .$$

Here, we’re essentially picking our best guess of the value of the nuisance parameters given a specified μ . The profile likelihood will obviously be useful in the limit of $\hat{\theta}$ being close to the true values of the nuisance parameters, but this isn’t guaranteed.

Marginalization: we simply integrate away the dependence on the nuisance parameters entirely:

$$p_{\text{marginal}}(x|\mu) = \int_{-\infty}^{+\infty} p(x|\mu, \theta)p(\theta)d\theta .$$

Note that this requires a specification of a prior pdf $p(\theta)$. Marginalizing is then a form of averaging of the likelihood and prior across the domain of θ . Despite this technically being a Bayesian procedure due to the specification of the prior, we’re free to use the resulting model in a frequentist way – this is just a model specification step.

2.2 Metrics of probability

2.2.1 Fisher information and the Cramér–Rao bound

A useful quantity in many ways is the **Fisher information matrix**. We can write the definition for an element of this matrix for a likelihood function $p(x; \theta)$ ($\theta = \{\theta_i\}$) as

$$\mathcal{I}(\theta)_{ij} = -\frac{\partial^2}{\partial \theta_i \partial \theta_j} \log p(x; \theta) .$$

We'll focus on the fact that you can extract *parameter uncertainty estimates* from this quantity. How? We turn to the Cramér–Rao bound, which states that if we have an unbiased estimator for the likelihood parameters $\hat{\theta}$, the Fisher information matrix $\mathcal{I}(\theta)$ satisfies

$$\Sigma_{\hat{\theta}^2} \geq [\mathcal{I}(\theta)]^{-1}, \quad (2.7)$$

where $\Sigma_{\hat{\theta}}^2$ is the covariance matrix for the fitted parameters $\hat{\theta}$. In the asymptotic limit, the maximum likelihood estimator will attain this lower bound, and satisfies

$$\sqrt{n}(\hat{\theta} - \theta) \rightarrow \text{Normal}(0, [\mathcal{I}(\theta)]^{-1})$$

for sample size n . A useful thing about this is that the diagonal elements of the inverse Fisher information will then correspond to the variances of the individual parameters, i.e. $[\mathcal{I}(\theta)]_{ii}^{-1} = \sigma_{\theta_i}^2$. There are also many other interesting quantities we can extract from this equivalence, including the *generalized variance*, which is the determinant of the covariance matrix (or determinant of the inverse Fisher information). These quantities will see a little use later on.

2.2.2 Kullback-Leibler divergence

The **Kullback-Leibler divergence** (KL divergence) is a commonly used quantity in machine learning and information theory to represent the “distance” between a probability distribution $p(x)$ and an estimation of that distribution $q(x)$. Related to things like entropy, it can be thought of as the loss of information from using q as an approximation to p . It's defined for continuous x as

$$D_{KL}(p(x)\|q(x)) = \int_{-\infty}^{\infty} p(x) \ln \frac{p(x)}{q(x)} dx . \quad (2.8)$$

One interesting thing to note is that this is not a distance in the typical sense, since it's an *asymmetric* number, i.e. $D_{KL}(p(x)\|q(x)) \neq D_{KL}(q(x)\|p(x))$.

2.3 Inference

Statistical inference can be viewed as the inverse of the data generating process. Let's look at an example.

Say that the Lorax created the Earth. Moreover, say that he did so by rolling a six-sided die, and putting the result of the die into a World Generating Machine, which merely requires a single number as input. As a neutral party that cannot confirm the Lorax's roll, but can definitely observe the outcome, we may wonder: assuming we have a model of the World Generating Machine, what number did the Lorax roll to produce all that we see around us today? Moreover, can we factor in our prior suspicion that a Lorax rolled a die to select a number at random?

Put in a more general way: given a parametrized model of the world around us, potential suspicions about the parameters themselves, and some data that could be described by that model, which values of the parameters could have produced the data? Moreover, is the model a good description of the data at all? Could another model have described the data more accurately? These type of questions fall within the umbrella of statistical inference.

Let us add a layer of specificity to our questions. The key inquiries that are typically dealt with through inference are:

- **Point estimation:** What value(s) of my model parameters best describe the data?
- **Interval estimation:** How can I specify a plausible range for my model parameters based on the data they attempt to describe? (One can obtain a symbiotic relation between interval and point estimation by viewing a point estimate as the limit of shrinking intervals)
- **Hypothesis testing:** Given a model of the data generating process, to what extent does it describe the data when...
 - ...compared to another model with different form?
 - ...compared to the same model with different parameters?
 - ...not being compared to any particular alternative? (this has the particular name of the *goodness-of-fit test*)

These questions are where the schools of probability see their strongest divide; whether we can assign probabilities to facts – e.g. what are the odds that neutrinos have masses – fundamentally alters the kind of question we can ask of our model/data. For example, instead of a point estimate of the neutrino masses, a Bayesian procedure could infer their *distribution* given the data (and some prior beliefs about their values), also termed the *posterior distribution*. Similarly, Bayesian intervals can say “what are the chances the true parameter value lies in this interval” (which frequentist procedures *can not determine*), and hypothesis testing can evaluate the probability of the hypothesis itself.

However, these Bayesian procedures undertake the weight of the specification of a prior distribution for all of these quantities, which will (in the limited data regime, a.k.a. real life) strongly affect the result. Moreover, the frequentist procedures are indeed still useful for making exact, even if convoluted, statements about the model in the presence of observed data.

A brief aside: you'll notice that the common thread throughout these statements is the *model*. As like many statistics-adjacent HEP researchers before me, I will emphasize that *the likelihood model is the most important ingredient for any inference procedure*. In the limit of a well-designed model and sufficient data, even a room full of the most polarized statisticians, hopelessly resigned to their particular school of thought, will agree on basic statements about the validity of a hypothesis. Even failing this, a Bayesian would not ignore a p -value of 0.9, and a frequentist would likewise raise their eyebrows at a flat or sharp posterior with low prior sensitivity. But since they both care about the model, any and all effort that could be spent arguing over inferencial philosophy may likely be better placed in talking to a domain expert for the problems you care about.

But enough with the aside, or I'll be subject to the same criticism of misplaced effort. Let's review the different methods that implement answers to our questions of inference.

2.3.1 Point estimation

Given a probability model $p(x|\mu)$ for data x and model parameters μ , the most common method of estimating parameter values compatible with observed data x_0 in the frequentist paradigm is the **maximum likelihood estimate** (MLE), defined as

$$\hat{\mu} = \operatorname{argmax}_{\mu} (p(x_0|\mu)) .$$

In practice, we calculate $\hat{\mu}$ with an optimization procedure, e.g. through the (L)BGFS algorithm for unconstrained optimization (Fletcher 1987). Since most optimization algorithms target minimization (purely conventional), we often frame this equivalently as

$$\hat{\mu} = \operatorname{argmin}_{\mu} (-2 \ln p(x_0|\mu)) .$$

The prefactor of 2 leads to some nice theoretical properties via Wilk's theorem, but that's a later discussion (the 2 doesn't matter for optimization purposes). We use calculate the MLE lot in HEP for a few reasons:

- It has a *Normal sampling distribution* in the asymptotic limit (so we can easily quote errors using a sample standard deviation)
- In the finite data regime, the MLE is effective for many distributions we care about (e.g. Normal, Poisson)

- Simple to understand and debug!

Other methods of point estimation could be as simple as quoting the *mode* (value with highest density), *median* (value that partitions the distribution into equal segments of probability), or *arithmetic mean* (sum of the data divided by the size of the data). These are more useful in the absence of a good probability model.

2.3.2 Confidence intervals

A significant part of my early PhD days was spent trying to understand the confidence interval. I will do my best to try and make you bang your head against the wall a little less than me (metaphorically, I hope).

We begin with some statistic of the observed data x . A confidence interval is then a statement about values of a model parameter μ for which the observed data is considered “*not extreme*”. Values of μ outside the interval are then those for which the observed data is “*extreme*”. We have a couple of ingredients to unpack here:

- How do we define a notion of “extreme” for the data?
- How do we construct the interval itself to satisfy this property (namely that the values of μ consistently treat x as extreme or not)?

For the first point, there’s a two-part answer: we need a way to order the data with a notion of extremity (rank it from least to most extreme), and then also determine the cutoff for which points are considered extreme or not. This cutoff isn’t going to be by value, but by *proportion*; we’ll place our yardstick such that all values of x considered *not extreme* contain the majority of the probability (area under $p(x|\mu)$). How much? That’s known as the **confidence level** (C.L.). Values considered *extreme* then occupy the other $1 - \text{C.L.}$ of the probability. We then determine those values of μ which produce distributions that satisfy this requirement *when the yardstick is in the same place as the observed data x_0* . We’ll see some examples of this below.

For 1-D x , we look at some simple orderings: - *Descending*: large x is not considered extreme, and small x is. The corresponding confidence interval is $[\mu_{\text{lower}}, +\infty]$, where μ_{lower} is known as a **lower limit** on μ . - *Ascending*: small x is now not extreme, but large x is. The corresponding confidence interval is $[-\infty, \mu_{\text{upper}}]$, where μ_{upper} is known as an **upper limit** on μ .

We can also look at a *central* ordering, which produces an interval that can be constructed at a given confidence level C.L. through calculating a lower and upper limit $[\mu_{\text{lower}}, \mu_{\text{upper}}]$, each with a confidence level of $1 - (1 - \text{C.L.})/2$ (which guarantees that the central interval contains C.L. of the probability).

Let’s make this concrete with an example: we’ll take the same distribution studied in (Cousins 2018) (Section 6.4), where we have a normal distribution with width parametrized as 1/5th of the mean:

$$x \sim \text{Normal}(\mu, \frac{\mu}{5}).$$

From here, we can examine the pdf (at $\mu = 10$ arbitrarily). We can also view the likelihood if we say we observed data $x_0 = 10$. Both are shown in Figure 2.2.

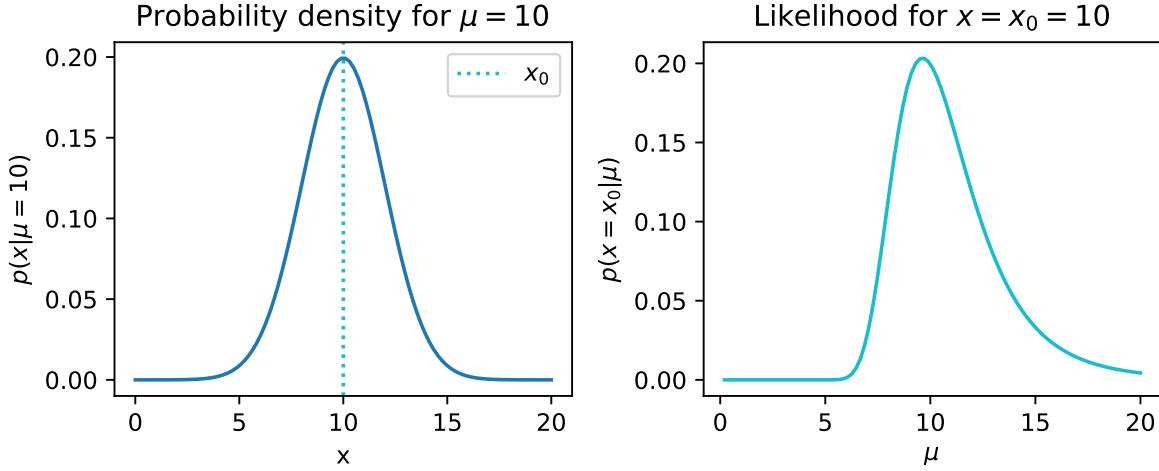


Figure 2.2: Probability density function and likelihood for different assumed values of x and μ .

Let's now use the aforementioned method to construct a central confidence interval for μ , at say a confidence level of 68.3%. We then divide up this confidence level into the lower and upper limits – each will be set with a confidence level of $1 - (1 - 0.683)/2 = 84.15\%$, such that the extreme data occupies one minus that amount (15.95%) of the probability on each side of the central interval, giving us back the desired 68.3% between the upper and lower limits.

Finding these limits can be viewed as an optimization problem: we just need to choose μ such that the area under $p(x|\mu)$ is equal to 84.15% *below* x_0 for lower limits, and *above* x_0 for upper limits. We can frame this objective using the cumulative density function – the cdf evaluated at x_0 must be equal to 0.843 for lower limits, and equal to 1-0.843 for upper limits. As this thesis focuses on methods relating to gradient descent, we can use this to find our central interval, by optimizing μ with respect to a mean-squared error loss between the cdf and the relevant probability share. Doing this for our example gives us the limits [8.332, 12.502] that form a central confidence interval for μ .

We can visualize the probability density for each of μ_{lower} and μ_{upper} , which should help cement the idea of capturing some amount of the probability up to x_0 based on an ordering of x :

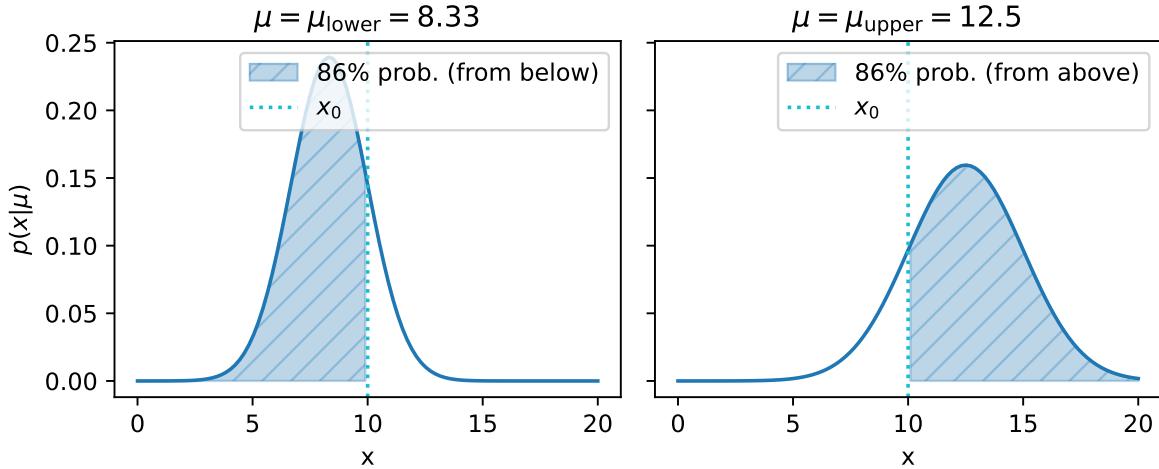


Figure 2.3: Probability density functions at both μ_{lower} and μ_{upper} , showing that the enclosed area under the curve at x_0 equals the desired amount as dictated by the confidence level.

Neyman construction

A different way to build confidence intervals (that generalizes to multiple dimensions) can be found in the form of the **Neyman construction**. Here, we start by constructing an *acceptance interval* for x . Given an ordering of x , a desired confidence level C.L., and a value of μ , an acceptance interval for x is defined such that the probability contained between $[x_1, x_2]$ is equal to C.L.. In equation form:

$$[x_1, x_2] \text{ s.t. } P(x \in [x_1, x_2] | \mu) = \text{C.L.}$$

The endpoints $[x_1, x_2]$ are well defined because we decided on an ordering for x (does not need to be central!), with any data outside these endpoints designated as “extreme” with respect to that ordering.

We can then draw the acceptance intervals for many values of μ . This can be visualized in a plot of μ against x as a set of horizontal lines in x corresponding to the acceptance intervals. How do we turn this into an interval on values of μ ? We just draw a vertical line corresponding to our observed data x_0 , and choose the values of μ that lie where the line intercepts the acceptance intervals for x . All of this is shown in Figure 2.4.

Even though the appearance of the plot in Figure 2.4 makes it look so, it is completely *not required that μ be 1-D!* For example, μ could easily have been 2-D here, and then the confidence interval in 2-D could still be constructed by the points at which the observed data (which would be the plane defined by $x_0 = 10$) meets the acceptance intervals, even if this stretches

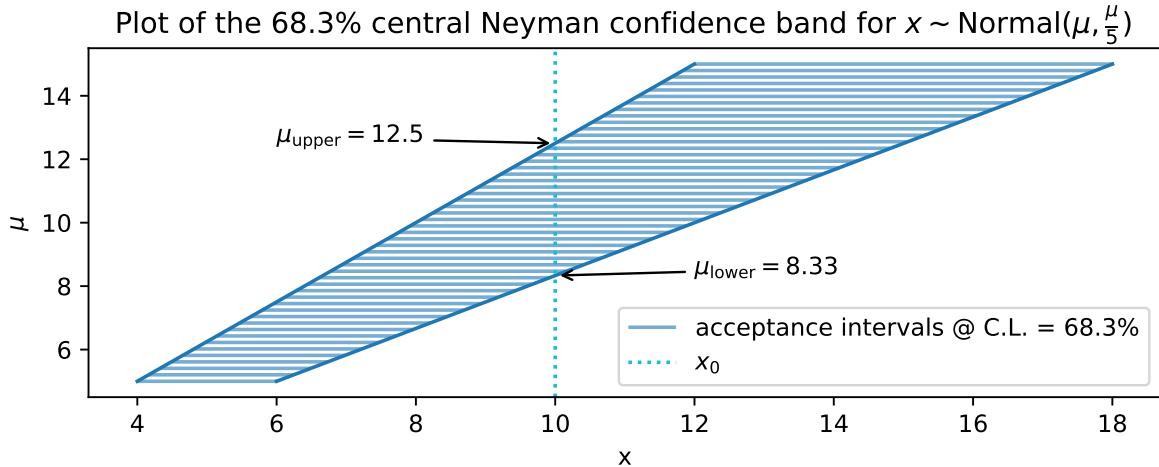


Figure 2.4: Neyman confidence band, showing both the overall envelop and explicit acceptance intervals in x . Also shows how one can then determine μ_{lower} and μ_{upper} at the intersection of the band and observed data x_0 .

out over other parameter dimensions. What happens if that multi-dimensional space becomes even larger, even if we don't care about some of the parameters? We'll look at new ordering principle for this.

Likelihood ratio ordering

A fourth ordering principle for the data was proposed by Feldman & Cousins in (Feldman and Cousins 1998), and is based on the likelihood ratio

$$R(x, \mu) = \frac{p(x|\mu)}{p(x|\hat{\mu})},$$

where $\hat{\mu}$ represents the best-fit value of μ . Commonly used in HEP, it appeals to intuition since there's then a correspondence between the notion of "extreme" and low probability density (relative to the maximum). Moreover, since it's a ratio, a change in variables from x to $f(x)$ would lead to the Jacobians cancelling in R , making this ordering invariant to a change of metric. We can construct intervals ordered by R through the Neyman method as above.

2.3.2.0.1 * Profiling

In the case where the likelihood parameters can be split into $[\mu, \theta]$, with θ representing nuisance parameters, we can make this interval construction more feasible by using the **profile likelihood ratio**:

$$\lambda(x, \mu) = \frac{p\left(x|\mu, \hat{\theta}(\mu)\right)}{p\left(x|\hat{\mu}, \hat{\theta}\right)}, \quad (2.9)$$

where $\hat{\theta}(\mu)$ represents the fitted value of θ when holding μ fixed. Doing this reduces the dimensionality of the parameter space to just those of which we're interested in (e.g. signal strength). However, coverage properties for intervals constructed in this way may vary, so need to have their sampling properties studied (see section 13 in (Cousins 2018)).

Coverage

Despite that a confidence interval is in values of μ , it's an inherently *data-dependent construct* – you'll get a different confidence interval for different observed data x_0 . The endpoints of the interval $[\mu_{\text{lower}}, \mu_{\text{upper}}]$ are consequently treated as random variables. The confidence level, then, is a property of the set of intervals that would be constructed over many experiments: if we sampled x from the true distribution many times with many experiments, and constructed a confidence interval using each sample with confidence level of 95%, then 95% of those intervals would contain (or **cover**) the true value of μ . The collection of these confidence intervals is called a **confidence set**, and we say that it has 95% **coverage**.

How do we know our confidence set has this property? Well, the Neyman confidence set has it by definition: if we think about just the single distribution at the true value μ_T , the Neyman procedure creates an acceptance interval such that the probability between $[x_1, x_2]$ is equal to the confidence level (say 95%). If we then do many experiments (i.e. sample $x \sim p(x|\mu_T)$), we know that 95% of the time, the dotted line representing the data point will lie within the acceptance interval of μ_T . Ah – this is exactly the requirement for μ_T to be included in our confidence interval! It then follows that 95% of the *intervals* constructed will then include the true value of μ , corresponding exactly to when the observed data lies within the acceptance interval for $\mu = \mu_T$.

This is all well and good, but may ring some alarm bells – we only have one interval in practice, right? Isn't there a chance that we draw data such that the confidence interval falls in the 5% that don't cover the true, unknown value of μ , and thereby *contradicting the distribution that produced the data point*?

In short, yes. But that doesn't mean confidence intervals are useless – a single 95% interval is overwhelmingly more likely to contain the true parameter value than not. Remember: we're always going to have inherent uncertainty on the statements we make on unknown true parameter values – this uncertainty is expressed as a probability distribution for Bayesian methods, and as a statement about sampling properties (results in the limit of many repeated experiments) for frequentist methods.

2.3.3 Frequentist hypothesis testing

Hypothesis testing gives us a framework to make qualitative statements about how extreme the observed data seems under a proposed theory, often in comparison to various alternatives. Note we use “extreme” in the same way as with confidence intervals, so we’re going to need to establish an ordering principle for the data. Let’s go into more detail.

Once again, we concern ourselves with a statistic of the data x and model parameters μ . Here we follow the conventions set out by Neyman (again) and Pearson in (Neyman and Pearson 1933), and start with the notion of a **null hypothesis** H_0 , which is the assumed default model for the data. One would often take this to be the Standard Model, for example. We then come up with an alternative hypothesis H_1 . In what way can H_0 and H_1 differ? We could have:

- Two totally separate probability models $p_1(x|\mu_1)$ and $p_2(x|\mu_2)$, which can differ in number of parameters and functional form
- A set of hypotheses within a probability model; $p(x|\mu)$ induces a family of hypotheses parametrized by μ , for instance, with any two values of μ potentially serving as H_0 and H_1

A hypothesis at a point (e.g. $p(x|\mu = 0)$) is known as a **simple hypothesis**, and a set of hypotheses (e.g. a second, unspecified model $p_2(x|\mu)$, or $p(x|\mu \neq 0)$) is known as a **composite hypothesis**. In HEP, we’re commonly testing a point null of $H_0 = \text{Standard Model}$ ($p(x|\mu = 0)$) against a composite alternative of $H_1 = \text{Something Else}$ ($p(x|\mu \neq 0)$). This poses a challenge from an optimality perspective that we’ll cover shortly.

So, how do we actually do the testing itself? We’ll need an ordering principle to rank data from least to most extreme. To do this, we usually concentrate on defining a good **test statistic** of the data $t(x)$, then fix an ordering of $t(x)$ ascending (but other orderings are possible, e.g. two-tailed tests are centrally ordered in $t(x)$). From there, we come up with a cutoff value t_c such that data with $t > t_c$ is seen as extreme. The proportion of the probability held by these extreme values is known as the **confidence level** or **test size** α .

Under *which distribution* is this ordering and designation of α performed? We do this with the pdf of the test statistic under the null hypothesis, $p(t(x)|H_0)$. Importantly, this distribution may not be known to us, and we may have to estimate it by sampling many values of $x \sim p(x|H_0)$, then calculate $t(x)$ for all of them, and estimate the density of the result. Moreover, without this distribution, we don’t know how to place our cutoff t_c so it contains a proportion α of the data considered most extreme!

One more thing we can deduce from the above: our statements on how extreme the observed data appears are *fundamentally under the assumption that H_0 is true*. Keep this in mind!

If the observed data x_0 falls in the extreme proportion of possible values, i.e. $t(x_0) > t_c$, we then say we *reject H_0* compared to H_1 . Note that this does *not mean we accept H_1 !* For that, we’d have to look at decision theory, which involves establishing the notion of probabilities for

H_0 and H_1 , which is beyond the scope of this frequentist testing framework (a more detailed discussion can be found in e.g. (Cousins 2018), Section 3.4).

So if our testing revolves around H_0 , where does the alternative H_1 come into play? We can see the presence of H_1 in commonly used orderings, such as the *likelihood ratio* of the two hypothesis: $t(x, \mu) = p(x|H_0)/p(x|H_1)$. Furthermore, we can define a measure of *error* in relation to H_1 : given H_1 is true, what's the probability of accepting H_0 , even when the data come from H_1 ? This quantity is known as β – a *powerful* test would have low β , i.e. often rejects H_0 in favour of H_1 when it is true, leading to the quantity $1 - \beta$ being known as the **power** of a test.

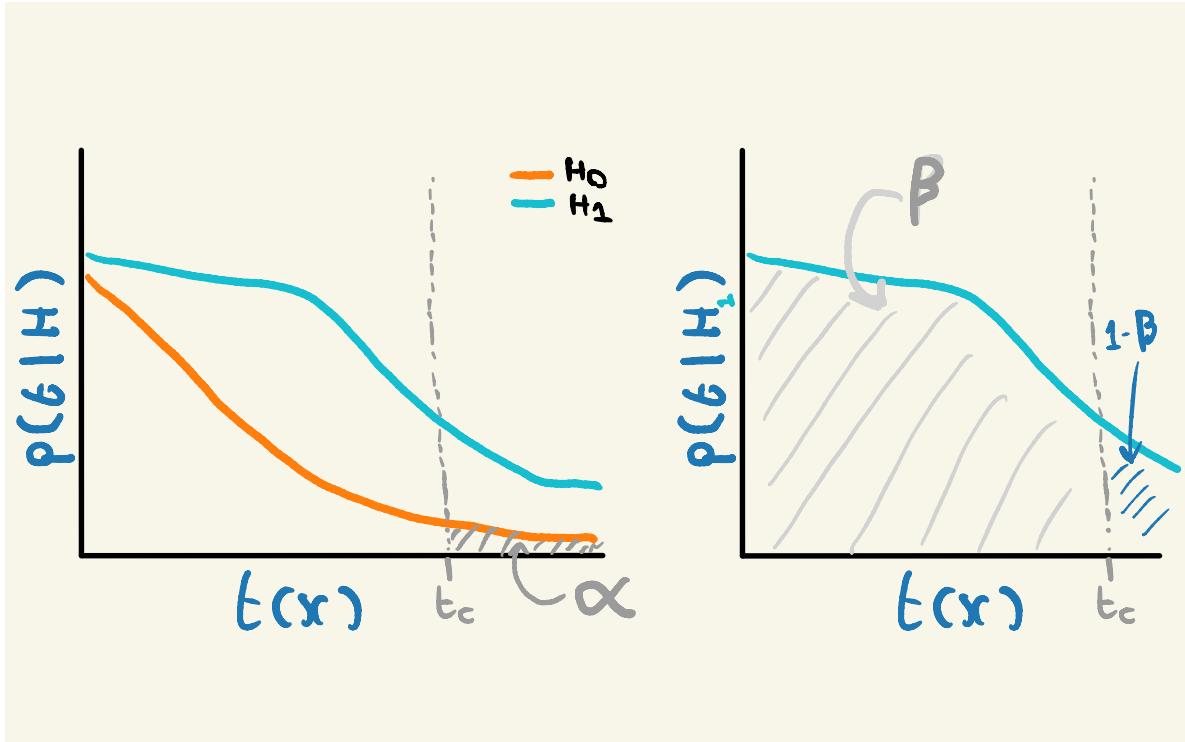


Figure 2.5: Visualization of a hypothesis test

When framing things in terms of error, we can see that the confidence level α also represents an error: *the probability of rejecting H_0 given that it's true*. Why? If the observed data was truly generated from H_0 , it will fall in the extreme proportion of the data exactly α of the time, since that's the way we designated the proportions to begin with. This would lead to the erroneous statement of rejecting H_0 (though we know this stops short of a *decision* on H_1). We can see a representation of both α and β in Figure 2.5.

The quantities α and β are often called *type-I* and *type-II* error respectively. I forget this all the time (in particular which type means what) so rarely use these names, but include them for completeness.

p-values

So we set up a test by choosing the size α , obtain the distribution for our chosen test statistic $t(x)$, and calculate the cutoff value t_c . What next? We'll take our observed data x_0 , calculate $t(x_0)$, and see if it lies past t_c . If so, we'll reject H_0 . If so, we'd maybe like to know by how much the data was incompatible with H_0 . This quantity is known as the *p-value*, and is just the area under $p(t(x)|H_0)$, i.e.

$$p_{x_0} = \int_{x_0}^{+\infty} p(t(x)|H_0)dx .$$

Note that the quantity p_x exists generally for x – this is just a rephrasing of the data into units that tell us how much of the test statistic distribution we're enclosing to the right under H_0 . p_{x_0} is then this statement for the observed data.

We can then rephrase a hypothesis test as rejecting H_0 when $p_{x_0} < \alpha$, and accepting H_0 otherwise. A low *p*-value is then a sign of low compatibility between the observed data and H_0 . (Here, my notation has come back to bite me... p_{x_0} is absolutely *not* the probability of x_0 !!!)

Optimality

What defines an optimal test? Well, α is specified prior to the test, so we're left with maximizing the *power* $1 - \beta$. The task then becomes: given α , choose a test statistic $t(x)$ such that the power $1 - \beta$ is maximized.

In the case where H_0 and H_1 are simple, the likelihood ratio is the optimal test statistic in the sense of power, which can be proved through the Neyman-Pearson Lemma (omitted here for the sake of brevity, though see a visual proof in (Cranmer 2020)).

When we have a composite hypothesis, things get trickier, since we've only worked out the best test statistic for two point hypotheses. Instead of most powerful test, we need to change our language: we want the *uniformly most powerful test* across the many point hypotheses contained within the composite hypothesis.

A proxy way to address this is the following: we know that the likelihood ratio is optimal for two point hypothesis. If we're testing a point null ($\mu = \mu_0$) against a composite alternative ($\mu \neq \mu_0$), we can represent the alternative through the *best-fit hypothesis to the observed data*, i.e. estimate $\hat{\mu}$ via maximum likelihood. We can then use the test statistic $p(x|\mu_0)/p(x|\hat{\mu})$. This is exactly analogous to the use of a likelihood ratio ordering in confidence intervals!

2.3.4 Duality between hypothesis test and intervals

It was probably hard to watch the number of times I defined “extreme” in this very specific way that seems to apply to both intervals and tests, without commenting on how they’re similar or different. That’s because they’re one-to-one in many ways!

Say we make a C.L. = 95% confidence interval of $[\mu_1, \mu_2]$ given an ordering principle/test statistic (e.g. likelihood ratio), a pdf $p(x|\mu)$, and some observed data x_0 . This interval contains all values of μ for which the observed data x_0 is deemed *not* extreme. Given the *same ordering principle*, a hypothesis test of some particular μ_0 asks: does x_0 lie in the extreme fraction of data $\alpha = 1 - \text{C.L.}$ when $\mu = \mu_0$? This is the *same thing* as asking: does μ_0 lie in the confidence interval $[\mu_1, \mu_2]$? If so, then the acceptance interval for $p(x|\mu_0)$ will be intersected by x_0 – this would *accept* H_0 in the testing framework, since x_0 under assumption of μ_0 is not considered extreme.

I hope this is clear enough, it took me a little while to see initially! One can then *invert a test* to produce a related confidence interval, which just means taking the set of μ that aren’t rejected in a test using the observed data:

$$\{\mu : t(x_0, \mu) < t_c\} = \text{confidence interval at C.L. of } 1 - \alpha .$$

2.3.5 Bayesian procedures

I won’t talk much about the Bayesian methodology here since I didn’t explicitly use it in my PhD, but it’s worth mentioning for contrast. Moreover, if you’re a student within HEP reading this, I don’t want to make it seem like there’s only one way of doing things – there are analyses that use these methods, and I think they should be explored more! See something like (Sivia and Skilling 2006) for a comprehensive introduction.

As I’ve mentioned a few times, the Bayesian interpretation of probability admits distributions for facts; one can ask “how likely is supersymmetry?” or “what’s the distribution for my signal strength?” These questions are often answered via use of Bayes theorem, which states that for probability distribution $p(\cdot)$, data x , and model parameters $\mu = \{\mu_1, \mu_2, \dots, \mu_n\}$,

$$p(\mu|x) = \frac{p(x|\mu)p(\mu)}{p(x)} .$$

We call $p(\mu|x)$ the joint **posterior** distribution of the parameters μ , since it reflects our updated beliefs post-data. We know about the likelihood $p(x|\mu)$, but $p(\mu)$ (the product of the individual distributions $p(\mu_i)$) is a new player in the game: these are the **prior** distributions for each parameter, called as such to reflect our prior belief in their distributions. We need to incorporate this information to perform inference using this paradigm, which is often a difficult task to

do faithfully (even when we want to claim ignorance). Finally, the normalizing factor $p(x)$ is termed the **model evidence**, and is obtained by marginalizing out the model parameters:

$$\text{Evidence} = \int_{\Omega} p(x|\mu) \times p(\mu) d\mu$$

over parameter domain Ω . Often, Bayesian computation only requires proportionality with respect to the parameters, so it's common to just think of the equation

$$\text{Posterior} \propto \text{Likelihood} \times \text{Priors}$$

as the defining equation of Bayesian inference, though the model evidence remains useful as a compatibility measure between data and likelihood.

One thing to note: Bayes theorem does not use the Bayesian definition of probability unless we decide to – it's derived from the axioms of probability, and is thus invariant of interpretation. Using this theorem in a Bayesian way only holds when we have a true but unknown quantity (e.g. μ) as the subject of our distribution, as is done here.

Armed with this equation, Bayesian procedures include:

- **Posterior estimation** (e.g. through Markov chain monte carlo and its variants)
 - Can then perform point estimation via *maximum a posteriori* (the mode of the posterior)
- **Credible intervals:** in contrast to confidence intervals where the endpoints are random variables, μ itself is now the random variable, and the interval is constructed such that it contains the true value μ_T with some allocated probability.
- **Hypothesis testing:** Bayesian hypothesis tests do exist, and involve the model evidence; I won't talk about them here.
- **Evidence estimation**, e.g. nested sampling (Skilling 2006), which also comes with a posterior estimate as a by-product.

3 Probability and Statistics, in practice

This section focuses on how fundamental statistical ideas are translated into meaningful physics insights. We'll look at common practice, and summarize the main components needed to set the scene for applications that involve building new ideas with these techniques.

My primary resources for this section were the seminal asymptotics paper (Cowan et al. 2011) and Kyle Cranmer's stats notes (Cranmer 2014).

3.1 Estimating distributions from data

Often we're not equipped with a way to describe some data we're interested in using a probability distribution. In that situation, it's useful to have a set of **density estimation** techniques within your toolkit. Here we go over a couple.

3.1.1 Histograms

Ah yes, the infamous histogram. Exceedingly simple by design, it approximates a data distribution through counting the number of data points that lie in a set of adjacent disjoint intervals, or **bins**. A histogram, then, is expressible as a set of counts and a set of bin edges. See some example histograms in Figure 3.1 to see how the binning can affect the overall envelope of the distribution.

The area under the histogram is equal to $\sum_{\text{bins } i} \text{count}_i \times \text{bin width}_i$; we can force this to unit area by dividing each term in the sum by the bin width and the total number of counts. This produces something that can be interpreted as a (discrete) probability density, which can be useful when looking at just the shape of the distribution, for instance.

3.1.1.1 Why histograms in HEP? {-}

I [asked this question on Twitter](#) because I was confused: the HEP analysis paradigm has the histogram as a central object, but why? The reasons I discovered are as follows:

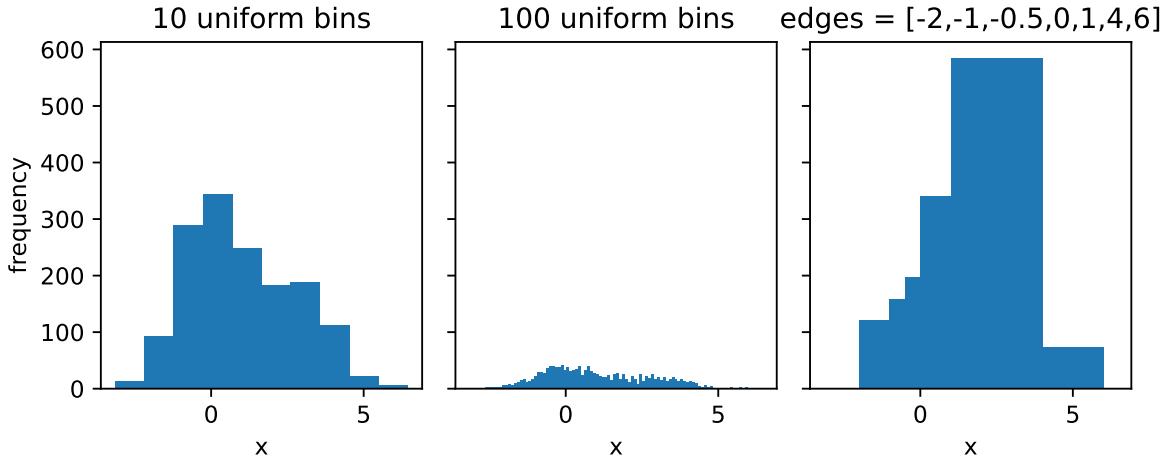


Figure 3.1: Histogram of some bi-modal data x , shown with different binnings.

- **Data structures:** the histogram has many benefits as a vessel to store data, e.g. their memory footprint is *independent of the size of the input data* – large numbers for the counts are still just single numbers! They also have effectively no cost to evaluate (you just look up the count number based on the bin)
- **Poisson modelling:** a simple and tractable way to model the likelihood of a collider physics process is with a Poisson-based likelihood function, which has an expected number of counts that is parametrized using templates from signal and background processes. When you make a histogram of your physics quantities, you can model it in this way through having one Poisson distribution per bin!

There was also more in that thread on ease parallel computation, the fact that histograms are good at respecting physical boundaries, and some birds-eye view perspectives on how things are (and could be) done in the field. Many thanks to Kyle Cranmer, Jim Pivarski, Stan Seibert, Nick Smith, and Pablo De Castro for contributing to that discussion – I encourage you to check out the thread!

3.1.2 Kernel density estimation

If you wanted a smooth distribution instead of a discrete one, the *kernel density estimate* (KDE) has you covered.

It's a pretty simple but powerful idea: for each data point, define some *kernel function* that uses the point as a centre (e.g. normal distribution). Then, the distribution of the data at a point x is equal to the average of the kernel functions evaluated at x .

There are many different choices of kernel function, each with their own tradeoffs, but the most common one in practice is indeed the standard normal distribution $\text{Normal}(0, 1)$. If

we specify the mean as the data, then there's one missing ingredient – the *width* of these distributions. That number is called the **bandwidth**, and controls the width of every kernel at once. Interestingly, the choice of bandwidth affects the resulting shape in general much more than the choice of kernel – see Figure 3.2 for some examples of the bandwidth's influence on the distribution.

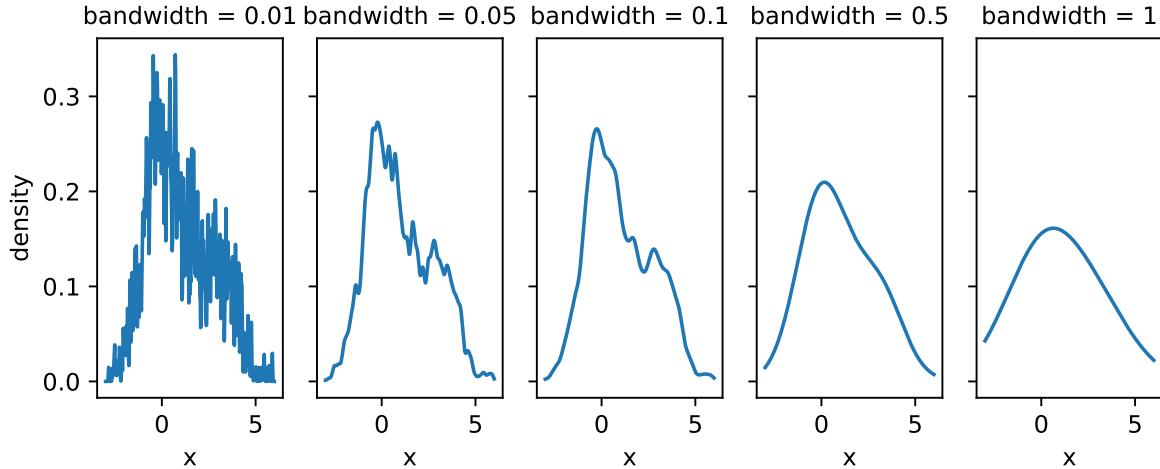


Figure 3.2: KDE of some bi-modal data x , shown with different bandwidths.

Some talk on a midpoint between KDEs and histograms will appear in the applications part of the thesis!

3.1.3 Fitting an existing distribution

If you have a decent idea on a distribution that may reasonably describe your data, you can simply perform a maximum-likelihood optimization to fit the parameters of the model to the data. One can even compose multiple distributions into a more complex likelihood. Not too much more to say about this, as it essentially comes under point estimation of a model parameter, which we talked about in the previous chapter!

3.1.4 Other data-driven methods

We'll talk more about these in the machine learning section, e.g. Gaussian processes and normalizing flows. These are generally reserved for when you need a little bit of extra work in order to get a robust result, or to go beyond 1-D and 2-D variables in a scalable way.

3.2 HistFactory: modelling nature as a set of counts

HistFactory (Cranmer et al. 2012) is by far the most common statistical modelling tool used for collider physics data analysis. It's known for being difficult to understand at first – if you've ever seen the full expression for the general likelihood, you'll have wondered if there was a need to extend the Greek alphabet to write down all the symbols that are used. Here, we'll take a slower and more gentle approach, building up the HistFactory likelihood piece-by-piece, until hopefully it's clear enough what's going on.

3.2.1 Baseline model for a chosen statistic

Given some (new) physics process exists, we may expect λ events to appear in our detector from that process. This number could come from e.g. simulating the physics process. It could also come from e.g. some data driven extrapolation method, but I'm going to call all of this simulation for the sake of the arguments below. The point is that we estimate it before looking at the important data in the region that would contain new physics.

So: say we run our detector, and we record n *independent* events. What's the likelihood of observing these n events with λ expected from simulation?

We know from the previous chapter that this is modelled well with a Poisson distribution:

$$p(n|\lambda) = \text{Poisson}(n|\lambda) . \quad (3.1)$$

Along with the overall number of events we recorded, we may pick some statistic of the data x that we choose to measure. That variable will have a distribution we can predict from simulation. How do we describe it?

We know that our data is divided into two categories: stuff that came from physics we're interested in (**signal**), and stuff that came from everything else (**background**). We can then say we have s signal events in our sample and b background events, with $s + b = \lambda$, our overall number of expected counts from simulation.

Each value of x that comes from a signal event can be viewed as a sample from the unknown signal distribution $f_s(x)$, and likewise for background $f_b(x)$. We can even think of any particular value we measured (e.g. x_0) as being “marked” with an extra number – either $f_s(x_0)$ if it came from signal, or $f_b(x_0)$ if it belongs to the background. This means that our overall distribution for the variable x is described by “ s ” much of $f_s(x)$, and “ b ”-much of $f_b(x)$, i.e. for any value of x , its density is then

$$p(x) = \frac{s f_s(x) + b f_b(x)}{s + b} , \quad (3.2)$$

where we choose to normalize by the total number of events $s + b$ to treat $p(x)$ as a proper density.

We can then model the whole dataset $\{x_i\}_{i=1}^n$ by multiplying the densities of all the individual events, since we assumed they were independent (otherwise we couldn't use the Poisson distribution!). We can then incorporate Equation 3.1 with Equation 3.2 through multiplication of the densities:

$$p(\{x_i\}_{i=1}^n) = \text{Poisson}(n|s+b) \prod_{i=1}^n \frac{sf_s(x_i) + bf_b(x_i)}{s+b}. \quad (3.3)$$

Notice that we don't have any free parameters right now – the counts s and b will be fixed from our physics simulation once we get around to it. But what if wanted to infer the amount of signal present in our data? How would we do that? We can accomplish this through a little trick: we can multiply the number of signal events s with an additional number μ that controls the overall **signal strength**. Estimating the value of μ would then tell us information about the amount of signal present in the data (assuming our model is accurate enough)!

We can now replace s with μs in Equation 3.3 to get

$$p(\{x_i\}_{i=1}^n|\mu) = \text{Poisson}(n|\mu s + b) \prod_{i=1}^n \frac{\mu sf_s(x_i) + bf_b(x_i)}{\mu s + b}. \quad (3.4)$$

In this formalism so far, we've kept things generalized to the “unknown” pdfs $f_s(x)$ and $f_b(x)$, but we don't actually have access to them. We can approximate them using a KDE or some other method, but it's more common to find us with a *histogram* for this representation (reasons for why are outlined in Section 3.1.1.1).

Say we histogram our simulated signal and background data with the same binning (not required to be uniform) that uses a number of bins k , giving us sets of counts $\mathbf{h}^{\text{sig}} = \{h_1^{\text{sig}}, h_2^{\text{sig}}, \dots, h_k^{\text{sig}}\}$ and $\mathbf{h}^{\text{bkg}} = \{h_1^{\text{bkg}}, h_2^{\text{bkg}}, \dots, h_k^{\text{bkg}}\}$. Recall from Section 3.1.1 that we can use these to approximate a density by normalizing with respect to bin width and number of events. Then, if we say a given value of x falls into some bin with index j , we can write that the density at x is approximated by the (normalized) count in that bin, for both signal and background separately:

$$f_s(x \in \text{bin } j) \approx \frac{h_j^{\text{sig}}}{s \times \text{width of bin } j}; \quad f_b(x \in \text{bin } j) \approx \frac{h_j^{\text{bkg}}}{b \times \text{width of bin } j}$$

From here, we can express Equation 3.4 as a product over bins j instead of events i :

$$p(\{n_j\}_{j=1}^k | \mu) = \text{Poisson}(n | \mu s + b) \prod_{j=1}^k \frac{\mu h_j^{\text{sig}} + h_j^{\text{bkg}}}{\mu s + b}.$$

Note that we've shifted from talking about values of x_i to bin counts n_j , where $\sum_{j=1}^k n_j = n$. These counts don't seem to appear in the likelihood yet, but we can make this explicit through the following relation¹:

$$\text{Poisson}(n | \mu s + b) \prod_{j=1}^k \frac{\mu h_j^{\text{sig}} + h_j^{\text{bkg}}}{\mu s + b} \propto \prod_{j=1}^k \text{Poisson}(n_j | \mu h_j^{\text{sig}} + h_j^{\text{bkg}}),$$

where the constant of proportionality is a factor involving factorials of the individual counts (also referred to as combinatorics). Since we don't care about the overall normalization when we do inference (e.g. the maximum likelihood value is independent of the scale, and the normalization cancels in a likelihood ratio), we will consider this proportionality as an equivalence.

These gymnastics have left us with the following likelihood:

$$p(\{n_j\}_{j=1}^k | \mu) = \prod_{j=1}^k \text{Poisson}(n_j | \mu h_j^{\text{sig}} + h_j^{\text{bkg}}), \quad (3.5)$$

which is simply a product over Poisson distribution for each bin within a histogram, where we expect a contribution of $\mu h_j^{\text{sig}} + h_j^{\text{bkg}}$ from each of signal and background respectively per bin j . This expression forms the core of the HistFactory approach.

3.2.2 Uncertainty modelling through nuisance parameters

Now, we'll extend the model from Equation 3.5 in a similar way to when we added μ to manipulate the signal scale, but this time, it's in order to be able to model uncertainties.

The origin of systematic uncertainties in simulation is this: we're uncertain as to the true values of the physics parameters that we should put into the simulator. Let's denote an example parameter with α . To quantify how varying α changes the likelihood in the ideal world, we would just include those parameters of the simulator within our likelihood model. However, this would require the ability to simulate data on-the-fly at any given value of the physics parameter, and then propagate that change all the way through our analysis selection requirements. This is difficult from both a practical and a computational perspective (the simulators we use are

¹This relation arises from noticing that $\lambda^n = \lambda^{\sum n_j} = \prod_j \lambda^{n_j}$, and using it to manipulate the Poisson on the left-hand side, amongst other things. We gloss over the full working, but I would like to include it if I have time (reading this means I probably didn't, but I do plan to release a blog post in future).

expensive to evaluate), plus it would have to be done for all the parameters we may want to model in this way. So what do we do instead? Here I give one example.

We may have a best prediction for α from studies carried out by e.g. a performance group in your collaboration that focuses on measuring α , but we'll also have some notion of uncertainty on that value, perhaps in the form of a distribution on α . An example procedure that we often do in this case is to just simulate our physics data at the best guess for that parameter α – we'll refer to this as the **nominal** value α_{nom} – and then also simulate data for values at $\alpha_{\text{nom}} + \sigma_\alpha = \alpha_{\text{up}}$ and $\alpha_{\text{nom}} - \sigma_\alpha = \alpha_{\text{down}}$, where σ_α is some notion of a standard deviation on α (e.g. calculated arithmetically on a sample or fitted as part of a normal distribution).

We're not restricted to the choice of α_{up} and α_{down} , but it's pretty commonplace as a quick way to get a rough idea of the influence of α on the histograms. And that's the point – we really only care about how varying α changes the resulting histogram for that process – either \mathbf{h}^{sig} or \mathbf{h}^{bkg} . We can then estimate the effect of α as a continuous change by some kind of *interpolation between the resulting histogram yields*. All of this results in the addition of as many extra factors as you like to Equation 3.5, which can be broken up into *multiplicative terms* and *additive terms* applied to both s and b , all of which serve to influence the shape and/or overall normalization of the resulting histogram.

3.2.3 Constraint terms

We discussed constraint terms briefly in Section 2.1.7, where we asserted that if a parameter α had some kind of external measurement that we wanted to incorporate into the *model* (not as a Bayesian prior), then we would have to include the likelihood function for that measurement $p(y|\alpha)$ in the full model, where y is the measured quantity that provides information about α . We would then multiply the likelihood in Equation 3.5 (after we added in our nuisance parameter α) by $p(y|\alpha)$ – the only problem is that we don't readily have access to this full likelihood. What we do instead is to introduce an approximate constraint that makes use of the provided information (e.g. up/down variations). The way this works is that we take a simple distribution like a standard normal, then choose our “units” such that , and the up/down variations are at $+/- 1$ standard deviation of, for example, a standard Normal distribution. This would then lead to multiplying Equation 3.5 by $\text{Normal}(y|\alpha, 1)$, where the nuisance parameter α is shared between both this part and the Poisson part of the overall likelihood.

To get some intuition for this: if $\hat{\alpha} \neq 0$ (which would correspond to being different to α_{nom}), the value of $\text{Normal}(y|\alpha, 1)$ will be lower than its maximum (since it's centered around 0), and will *penalize* the likelihood for contradicting the information on our best guess of α , i.e. we got a lower likelihood than we could have if we agreed more with our previous information on α .

3.3 Hypothesis testing and asymptotic formulae in HEP

In Section 2.3.3, which covered frequentist hypothesis tests, we noted that we don't necessarily have access to the *sampling distribution* of the test statistic $p(t(x)|H_0)$ given a particular null hypothesis H_0 , which is the key quantity we need to be able to set our cutoff value for the test. One way to estimate $p(t(x)|H_0)$ is to simply calculate $t(x)$ for many samples $x \sim p(x|H_0)$, and build up the distribution empirically. However, there exist some choices of $t(x)$ that give us *asymptotic guarantees* as to the form of $p(t(x)|H_0)$, i.e. we can fairly reliably know its shape as long as we have a decent enough sample size of x .

One of these choices that we've seen a couple times already is the likelihood ratio between a point null at μ and a composite alternative represented by the maximum likelihood point $\hat{\mu}$:

$$R(x, \mu) = \frac{p(x|\mu)}{p(x|\hat{\mu})}.$$

We'll likely have to deal with nuisance parameters in the likelihood, for which we extend this as shown in Equation 2.9 to:

$$\lambda(x, \mu) = \frac{p\left(x|\mu, \hat{\theta}(\mu)\right)}{p\left(x|\hat{\mu}, \hat{\theta}\right)},$$

where we recall that $\hat{\theta}(\mu)$ represents fitting the value of θ while holding μ fixed at its value from the input to λ .

This quantity (or $-2 \ln$ of it at least) forms the basis of all test statistics that we use in tests for the discovery of a new particle, or for setting a limit on a physical quantity (e.g. a particle mass or process cross-section).

3.3.1 Sampling distributions for $-2 \ln \lambda$

The first result we'll exploit to our advantage is that of Wald (1943), who showed that we can relate $\lambda(x, \mu)$ with the maximum likelihood estimate $\hat{\mu}$ in the following way:

$$-2 \ln \lambda(x, \mu) = \left(\frac{\mu - \hat{\mu}(x)}{\sigma_{\hat{\mu}}} \right)^2 + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right), \quad (3.6)$$

where $\sigma_{\hat{\mu}}$ is the standard deviation of $\hat{\mu}(x)$, which will tend to a normal distribution of this width with sufficient data (and is assumed to do so here), and N is our data size. This equation is known as **Wald's relation**. Note that this is just a quadratic in $\hat{\mu}(x)$ – the plot

of $-2 \ln \lambda(x, \mu)$ vs $\hat{\mu}(x)$ will be a parabola (to the extent that we can neglect the $\mathcal{O}(1/\sqrt{N})$ term). The uncertainty $\sigma_{\hat{\mu}}$ is an important quantity that we'll talk about in later sections after doing some groundwork.

Another interesting result is that since we're already incorporating nuisance parameters within λ , the shape of the test statistic against $\hat{\mu}(x)$ will follow this relation independent of the value of the nuisance parameters.

How do we go from here to $p(-2 \ln \lambda(x, \mu) | H_0)$? We can take another look at Equation 3.6 and notice that the RHS has the quantity $(\mu - \hat{\mu}(x))/\sigma_{\hat{\mu}}$ all squared. In the large sample size limit (asymptotically), $\hat{\mu}(x)$ is normally distributed around μ with width $\sigma_{\hat{\mu}}$, meaning that $(\mu - \hat{\mu}(x))/\sigma_{\hat{\mu}}$ follows a standard normal distribution! So if we have a standard normally distributed variable squared, i.e. $\lambda(x, \mu)$, we have a χ^2 distribution with one degree of freedom!

This is a powerful result. Let's apply it for our case of interest, which is the test statistic distribution evaluated at the null, $-2 \ln \lambda(x, \mu_0)$. Neglecting the $\mathcal{O}(1/\sqrt{N})$ term for now, we write

$$-2 \ln \lambda(x, \mu_0) = \left(\frac{\mu_0 - \hat{\mu}(x)}{\sigma_{\hat{\mu}}} \right)^2. \quad (3.7)$$

We can then say that, under the assumption of H_0 (i.e. assuming $x \sim p(x|\mu_0)$), the MLE $\hat{\mu}$ will be normally distributed around μ_0 , and $-2 \ln \lambda(x, \mu_0)$ then follows a χ^2 distribution with one degree of freedom. This is known as **Wilks' theorem** Wilks (1938), and gives us access to the sampling distribution we need for hypothesis testing.

What happens when the value of μ in the data set is different to μ_0 , and instead is some value μ' ? The result from Wald in Equation 3.6 allows us to generalize the result from Wilks, where we instead find that have a *non-central chi-square distribution* with one degree of freedom, written as $\chi^2(\Lambda)$, which is determined by the non-centrality parameter Λ , given by

$$\Lambda = \left(\frac{\mu_0 - \mu'}{\sigma_{\hat{\mu}}} \right)^2. \quad (3.8)$$

We can see that when we're back in the regime of $\mu' = \mu_0$, the non-centrality parameter is 0, which makes the distribution a regular (central) chi-square, as in Equation 3.7. This result will be particularly useful in later sections.

Just to recap notation here, since we're accumulating a few forms of μ :

- μ_0 is the value of μ being *tested as the null hypothesis*, with the alternative being $\mu \neq \mu_0$.
- $\hat{\mu}$ is the value *fitted to the observed data* by maximum likelihood.
- μ' is the *assumed* value of μ present in the data itself.

The reason to make the distinction between μ_0 and μ' in particular is that we may not always want the distribution of the test statistic under the null. An example for this is that when we report the expected discovery significance, we're testing a null of $\mu_0 = 0$, but would like to see if we can discover the signal assuming it exists in the data, which would mean we want $p(-2 \ln \lambda(x, \mu_0) | \mu')$, with μ' usually being taken as the nominal value of 1 for the signal hypothesis. For that, we're able to leverage Wald's result of having a non-central chi-squared distribution, with the non-centrality parameter given as in Equation 3.8.

3.3.2 The catalog of test statistics

The results we showed in the previous section hold for a test statistic of $-2 \ln \lambda(x, \mu)$. In practice, we tend to use some slight variations on this, depending on the physics task we want to undertake. Here are some examples.

Discovery

When we are searching to **discover** a new physics process, we will test using

$$q_0(x) = \begin{cases} -2 \ln \lambda(x, 0) & \text{if } \hat{\mu} \geq 0, \\ 0 & \text{if } \hat{\mu} < 0 \end{cases}, \quad (3.9)$$

where we have a null hypothesis of $\mu_0 = 0$, i.e. we test the background-only model. The reason we set $q_0 = 0$ when $\hat{\mu} < 0$ is that this would imply that the MLE for the expected number of events is even smaller than the nominal background, so we assume no signal is present. That means rejection of $\mu = 0$ would then only indicate a positive signal strength $\mu > 0$, indicating the potential presence of some amount of signal.

Upper limit setting

We can also use our hypothesis test as a mechanism to set an **exclusion limit** on the signal strength μ , which is conventionally done through an upper limit, as defined in Section 2.3.2². For this, we again turn to $-2 \ln \lambda(x, \mu)$, but only for fitted values of μ that are *less* than the value of μ being tested. The reason for this is that data with $\hat{\mu}$ *above* our tested value would make it even more signal-like than the null, which for the purposes of bounding μ from above, would not be desirable to be in the “extreme” region of the data, i.e. in the rejection area for the hypothesis test. We can circumvent this by setting the test statistic to 0 for $\hat{\mu} > \mu$, giving us the expression

²We could equally well look at other ordering choices, e.g. a central interval for μ .

$$q_\mu(x) = \begin{cases} -2 \ln \lambda(x, \mu) & \text{if } \hat{\mu} \leq \mu, \\ 0 & \text{if } \hat{\mu} > \mu \end{cases} . \quad (3.10)$$

Alternative test statistics exist in both cases (denoted by \tilde{q}_μ) for when the model disallows negative values of μ . These are not discussed here, but only require minor changes to the definitions of Equation 3.9 and Equation 3.10.

3.4 Asymptotic formulae for simple p -value calculations

The formulae presented here all stem from the result by Wald in Equation 3.6; they will be stated without lengthy derivation, but the working is mostly algebraic in nature, and builds upon the fact that we neglect the $\mathcal{O}(1/\sqrt{N})$ term in that equation³.

We start with the fact that the p -value (denoted p_μ here to highlight the selection of the null hypotheses) from any hypothesis test that we plan to do here can be written as

$$p_\mu = 1 - F(t(x, \mu) | \mu') ,$$

where $F(t(x, \mu) | \mu')$ is the *cumulative distribution function* for our test statistic $t(x, \mu)$, some chosen value of μ as our point null, and an assumed signal strength μ' in the data.

As in Section 3.3.2, when trying to discover a signal, we choose the test statistic $t(x, \mu) = q_0$. In this case, the cumulative distribution $F(q_0 | \mu')$ can be derived from the results in Section 3.3.1, which comes out to be

$$F(q_0 | \mu') = \Phi \left(\sqrt{q_0} - \frac{\mu'}{\sigma_{\hat{\mu}}} \right) ,$$

where Φ is the cumulative distribution of the standard Normal distribution. In the case that the data is drawn from the null distribution ($\mu' = 0$), this reduces to

$$F(q_0 | \mu') = \Phi(\sqrt{q_0}) , \quad (3.11)$$

meaning our p -value is then

$$p_0 = 1 - \Phi(\sqrt{q_0}) .$$

³In Cowan et al. (2011), they show that N need only be 10 or so for this to work well in their experiments.

For upper limits, we're switching to using q_μ as our test statistic. Similarly to q_0 , this leads to the cumulative distribution

$$F(q_\mu | \mu') = \Phi\left(\sqrt{q_\mu} - \frac{\mu - \mu'}{\sigma_{\hat{\mu}}}\right) ,$$

which, if the data is from the null ($\mu = \mu'$), leads to the same result as Equation 3.11:

$$F(q_\mu | \mu') = \Phi(\sqrt{q_\mu}) .$$

Our p -value is then just

$$p_\mu = 1 - \Phi(\sqrt{q_\mu}) . \quad (3.12)$$

These simple formulae underpin pretty much all major data analysis at the Large Hadron Collider – we too will make use of them later on.

3.5 The Asimov dataset and $\sigma_{\hat{\mu}}$

In Cowan et al. (2011), they proposed the notion of the **Asimov dataset** $x_A(\mu')$, which is defined for a given value of the signal strength μ' as the dataset that would cause the fitted value $\hat{\mu}$ to equal μ' (and also some value of the nuisances θ to equal θ' , just to fully specify the parameters). As a simple example, assuming no background uncertainty in the model, this would just be the expected counts at $\mu = \mu'$, i.e. $\mu' s + b$.

This may not appear that useful at first, but we can use this in conjunction with the results from Section 3.3 to produce some simple formulae that let us perform hypothesis tests without much computation at all. We start by remembering the result from Wald in Equation 3.6, which tells us

$$-2 \ln \lambda(x, \mu_0) \approx \left(\frac{\mu_0 - \hat{\mu}(x)}{\sigma_{\hat{\mu}}} \right)^2 .$$

Evaluating this at the Asimov dataset:

$$-2 \ln \lambda(x_A(\mu'), \mu_0) \approx \left(\frac{\mu_0 - \mu'}{\sigma_{\hat{\mu}}} \right)^2 ,$$

since, by definition of x_A , $\hat{\mu} = \mu'$. This is exactly the definition of the non-centrality parameter Λ from Equation 3.8! So using this specific construction of the Asimov dataset, we can get an

estimate of Λ , which characterizes the *general* distribution of $-2 \ln \lambda(x, \mu_0)$. Moreover, we can simply rearrange this equation to get

$$\sigma_{\hat{\mu}}^2 \approx -\frac{(\mu_0 - \mu')^2}{2 \ln \lambda(x_A(\mu'), \mu_0)} , \quad (3.13)$$

which is an estimate of the variance that characterizes the Normal distribution of $\hat{\mu}$, irrespective of the value it often takes in practice (this will just shift the mean).

Another way to estimate $\sigma_{\hat{\mu}}^2$ is using the Fisher information matrix of the HistFactory likelihood as in Section 2.2.1, where the diagonal term in its inverse corresponding to the index in the likelihood for μ would provide such an estimate, under similar requirements for the asymptotic unbiasedness of the maximum likelihood estimate $\hat{\mu}$. Both approaches are perfectly valid, though Cowan et al. (2011) claim that Equation 3.13 generally performed better in their experiments.

3.6 The CL_s quantity

When setting upper limits, instead of calculating p -values as in Equation 3.12, the ATLAS experiment mainly uses a modification of p_μ that divides by the *power of the test* $1 - \beta$. Originally proposed in (Read 2002), in which it was termed CL_s , the quantity is defined as the ratio

$$\text{CL}_s = \frac{p_\mu}{1 - p_{\mu=0}} ,$$

where $p_{\mu=0}$ is the p -value for the background-only hypotheses, which corresponds to the type-II error β , since $\mu = 0$ faithfully represents the alternative when setting limits. At first glance, there's no statistically obvious interpretation of a ratio of two p -values, but it does have the desirable property that, for tests with low power (i.e. low sensitivity to the alternative model), the CL_s value will be higher than the associated p -value, and we have less chance to erroneously reject the null when we don't have good test power to begin with.

4 Gradient descent

4.1 Introduction

Moving forward with the groundwork from the previous section on automatic differentiation, we'll dive into how this enables a particular learning procedure called *gradient descent*. We'll explore what that means, then apply this to a few different scenarios to demonstrate its utility, along with highlighting some more intelligent versions that have arisen as a by-product of the recent deep learning revolution. Importantly, this will also set the stage to show the main mechanism for how neural networks are able to train.

Say we have a ball on a hill, and we wanted to roll it down. How would you go about this task? Well, I imagine you'd probably just give it some initial kick, and then let gravity do the rest. Alright then – let's take away gravity. What then? Look for the bottom of the hill and try to push it there? But what if you can't see the hill itself? This is the situation we find ourselves in when trying to optimize a workflow. We're able to see what point we're at during optimization, but we don't know where the bottom of the hill is (minimum of our objective), or what the surrounding landscape looks like (could be very expensive to scan over the space).

Ah, but here's a trick: if we can see where we are at one point on the hill, we can determine the way the slope goes that we're standing on. If the slope points up, we'll want to push the ball in the opposite direction to go down. Then, we're guaranteed to at least get *nearer* the bottom of the hill. But by how much do we push the ball?

If the ball is close to the bottom of the hill, you could imagine that the ground starts getting flatter, which would make the magnitude of the slope less. Likewise, if the slope is steep, we know we're probably not at the bottom yet, so we should move a reasonable amount. We can then just move *proportionally to the magnitude of the slope*.

To write this out in equation form: given the horizontal position on the hill x_i , and the vertical position y_i , we propose to move to a new point x_{i+1} in proportion to the slope at the point that we're on, i.e.

$$x_{i+1} = x_i - \alpha \frac{\Delta y_i}{\Delta x_i},$$

where α is the constant of proportionality that we're free to choose (also called the **learning rate**, since it modifies the step size we take), and Δ is a small change that we assume we can

calculate. Take note of the minus sign – this is us trying to move in the *opposite direction to the slope* at x_i .

Instead of assuming we can numerically calculate the small change Δ , we actually already have a way to calculate a small change at a point from calculus: the derivative! So if we take y as a function of x , then we can replace the deltas with the gradient of $y(x)$ evaluated at our current point x_i , leaving us with

$$x_{i+1} = x_i - \alpha \frac{\partial y(x_i)}{\partial x_i} . \quad (4.1)$$

Equation 4.2 is the equation for gradient descent, and is probably the most important equation in the whole thesis, since it enables all of the downstream applications I'll talk about later. It's also the mechanism that enables most artificial intelligence systems to learn.

To reframe this equation one more time through the lens of optimization: given an **objective function** or **loss function** L with parameters φ that defines a goal relative to data d (so $L = L(\varphi, d)$), we can use *gradient descent* to update the parameters φ such that we minimize the objective evaluated at d :

$$\varphi_{i+1} = \varphi_i - \alpha \frac{\partial L(\varphi_i, d)}{\partial \varphi_i} . \quad (4.2)$$

See a pictorial demonstration of this rule in Figure 4.1.

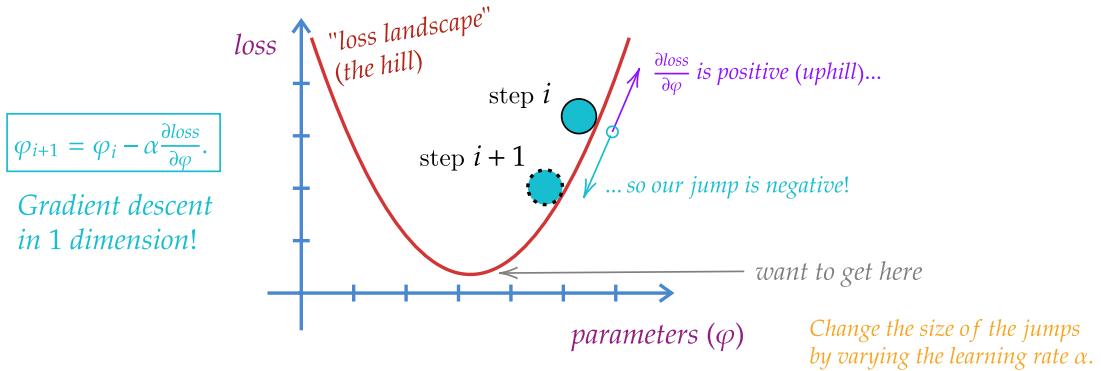


Figure 4.1: Gradient descent is more easily digestible when considering it as rolling a ball down a hill, but you need to play the role of gravity.

We're now specifying the data d because we want to give meaning to the vertical position in the hill: it's some quantity that's assessing the quality of our workflow with respect to some data from the real world d , given that we're using parameters φ_i . In practice this may be a

small subset of the dataset that we draw at random, since we can't computationally do this update on the whole data set due to memory restrictions on the device we run this on.

A key point to highlight: this mechanism only works if L is differentiable with respect to φ , otherwise we won't be able to calculate its gradient. This restriction may look tame for common objectives, which tend to involve simple algebraic expressions involving the output of a neural network, which is already a differentiable function. However, if we want to add domain knowledge to our loss function, we may end up discovering that not everything we want to calculate has a well-defined gradient. There are various ways to get around this, including the use of surrogate operations that are **relaxed** (jargon for differentiable) versions of their non-differentiable counterparts. We'll look at this in more detail when we study applications of this nature.

Let's look at an example of gradient descent in action.

4.1.1 Example: maximum likelihood estimation

Say we have some example data drawn from a bi-modal probability distribution that's somewhat normal-looking, like in Figure 4.2. We may want to try and model this with a normal distribution, but how do we choose the parameters? We can fit them to the data using maximum likelihood estimation, discussed further in Section 2.3.1. The basic idea is that, given a probability distribution p with parameters μ , we want to calculate

$$\hat{\mu} = \operatorname{argmin}_{\mu} (-2 \ln p(x|\mu)) ,$$

given some observed data x . In other words, we want to find the value of μ such that we minimize the negative log-likelihood. We can do this via gradient descent!

Using the update rule in Equation 4.2 with L as the negative log-likelihood and (μ, σ) playing the role of φ , we can run gradient descent for some number of steps until we reach a result that converges within some tolerance. We'll have to pick some initial value to start for each parameter – here we use 1 for each. In the implementation, we're using the automatic differentiation framework JAX (Bradbury et al. (2018)) to calculate the gradient of the objective (online viewers can expand the code block above the figure to see the details). This gives us a result in Figure 4.3, which isn't particularly great in my opinion.

Pretending we didn't know that the data came from a mixture of normal distributions, we can make a more sophisticated model, e.g.

$$p(x|\mu_1, \sigma_1, \mu_2, \sigma_2) = \frac{1}{2} \text{Normal}(\mu_1, \sigma_1) + \frac{1}{2} \text{Normal}(\mu_2, \sigma_2) .$$

We can then simultaneously optimize $\mu_1, \sigma_1, \mu_2, \sigma_2$ in exactly the same way, with no modification to the procedure other than using the new likelihood as the loss function. Doing this yields the

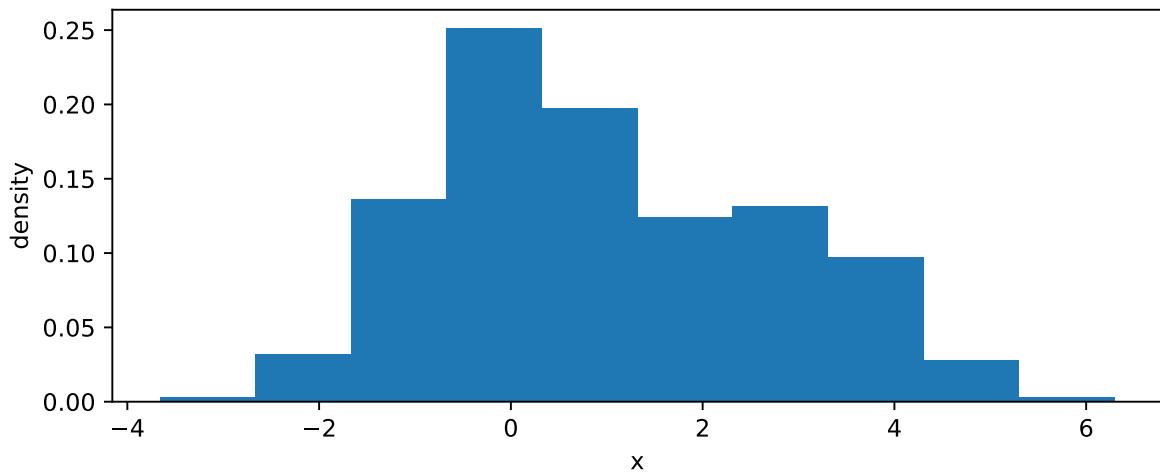


Figure 4.2: Example data produced using two normal distributions in unequal amounts. One is centered on 3, and the other on 0, both with unit standard deviation.

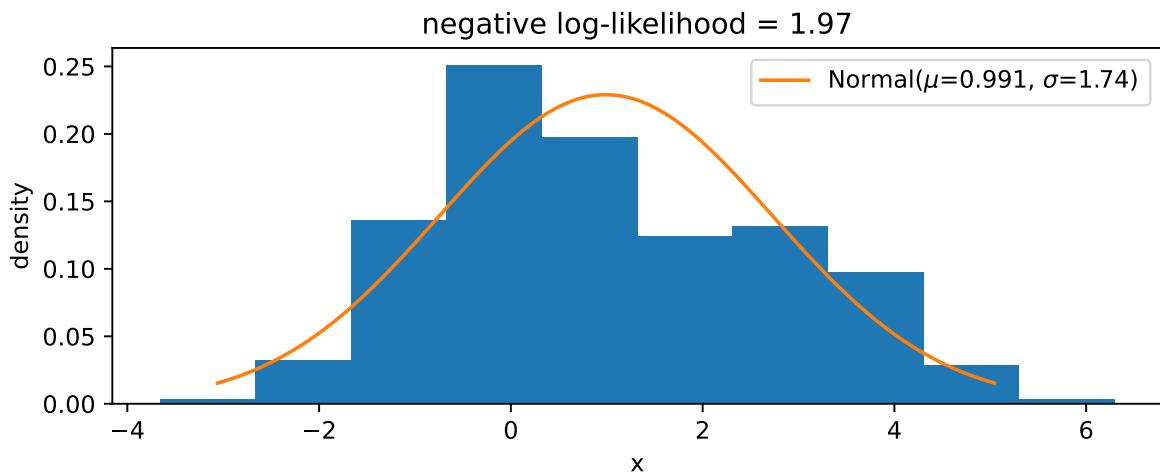


Figure 4.3: A single normal distribution fitted to the data in Figure 4.2 using gradient descent.

distribution in Figure 4.4. We can tell that the shape of the distribution is represented better here, which is also indicated by the lower negative log-likelihood than in the case of the single normal distribution. Since we forced the proportions of the mixture to be half and half, the lower second peak is modelled through a wider normal distribution to match the height of the second, smaller mode.

Interestingly, if we use 1 as the init for every parameter, we recover the solution from Figure 4.3, so we have to make sure there's a little mutual variation in the starting values so that the gradients push the different μ and σ values from different positions, allowing the second mode to be discovered. This demonstrates the behavior of gradient descent to move to some *local* minimum of the objective, and won't always converge to something optimal or intuitive.

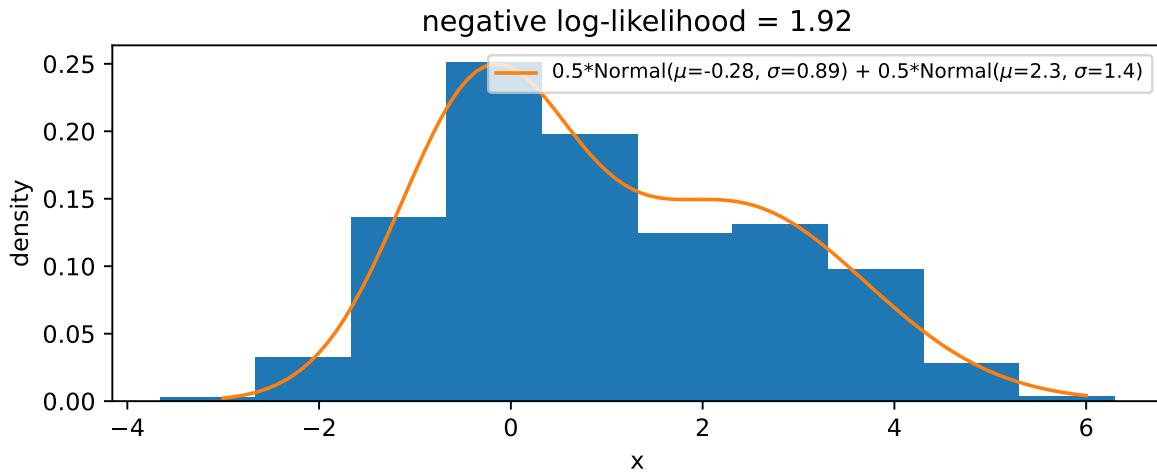


Figure 4.4: A mixture of two normal distributions fitted to the data in Figure 4.2 using gradient descent.

4.2 Mini-batching and stochastic gradients

In reality, we're not generally able to update our parameters using gradients computed over all our data at once in one batch, since that data may not fit on the device we're using to compute the program. We'd like to do this if we truly want to calculate the expectation of the gradient (in practice, the empirical mean) across all the training data we have, which has some convergence guarantees for arriving at a local minimum. Instead, we often split our data up into **minibatches**, which are fixed-size partitions of the data, typically randomly selected¹.

¹There's a funny issue to do with the notion of randomly selecting here; if we select *with replacement*, then we're sampling i.i.d. uniform random variables. This makes the theory of analyzing the performance much neater. But in practice, we never do this, and just shuffle the data and stream it, making it non-i.i.d., and therefore more difficult to analyze.

When we have seen enough batches such that we cover all the available training data, that number of steps is known as an **epoch**. This gives rise to the notion of the **batch size** – the size of each partition – which then inherently decides how many steps an epoch will take (smaller batch size = more steps and vice-versa).

An extreme version of splitting up into batches is **stochastic gradient descent**, which is just setting the batch size to 1. Gradients computed in this way will have very high variance as the name suggests, since parameter updates would be based on the performance on each individual training example. Surprisingly though, this high variance of the gradients can often help when wanting to explore the loss landscape more, and may help in jumping to new local minima that batch gradient descent may ignore.

4.3 Speeding up convergence: different optimizer types

To improve upon the rate of convergence in minibatch gradient descent, several variants have been proposed that incorporate additional information to make the gradient update. The methods are generally referred to as **optimizers** – we'll cover just a couple of the more common ones here.

4.3.1 Momentum

What happens when we're in a ravine during optimization, i.e. a local minimum with two steep slopes on either side in one dimension? Without modification, gradient descent will typically bounce between the ravines: we're moving in the downward direction, and with a larger step size since the slope is steep. How may we help this converge easier? Well, we could of course modify the learning rate in an adaptive fashion to try to dampen this oscillation about a minimum in a ravine. Something else that is done is to incorporate some amount (γ) of the *previous update step*, which we can write with a modified update rule through a placeholder variable v , defined recursively:

$$v_i = \gamma v_{i-1} + \alpha \frac{\partial L(\varphi_i, d)}{\partial \varphi_i}; \quad \varphi_{i+1} = \varphi_i - v_i .$$

To give some intuition as to what's happening here, we note that there's still a standard gradient update rule in there, but we're also “speeding up” the update by an amount γv_{i-1} , meaning if we did a large update previously, then we'll go even further this time. The analogy here is really still a ball rolling down a hill, but we're compounding speed just like gravity would make us do in real life. Moreover, if the previous update had a different sign for the gradient (travelling in the opposite direction), we'll actually be *slowed* by γv_{i-1} , which will prevent these types of oscillating situations bouncing between two steep slopes. This is termed gradient descent with **momentum**; I don't know if this was where it was originally proposed,

but many seem to cite (Qian 1999), despite it opening with “A momentum term is usually used in...”.

4.3.2 Adagrad

We return to the idea of *adaptive learning rates*. In the multi-dimensional parameter setting (could even be billions if we’re looking at neural networks), some parameters will have higher importance than others, i.e. the loss landscape could be flat in some dimensions, and convex in others. However, there could be parameters that are locally flat in some region, but have more interesting structure at a distance far from that region, or perhaps at least have structure that is more widely spread out. This could happen if that parameter is responsible for information relating to a sparse feature, for instance. If the learning rate makes the stepsize small in comparison to this distance, then we’ll never explore that structure well. This then gives rise to the notion of adapting the learning rate on a per-parameter basis to aid more efficient exploration of the loss landscape in search of a local minimum.

Adagrad (shorthand for “adaptive gradient”) is a method that endeavors to tackle this issue. It scales the learning rate for each parameter in such a way as to increase the step size for parameters in which we have moved less, and decrease it for those in which we have moved more. Specifically, it scales the learning rate by the inverse of the sum of the (squared) gradients. Denoting the gradient of one example parameter $\varphi^{(1)}$ at step i as $g_i^{(1)}$, we can write the update step for that parameter as

$$\varphi_{i+1}^{(1)} = \varphi_i^{(1)} + \Delta\varphi_i^{(1)}; \quad \Delta\varphi_i^{(1)} = -\frac{\alpha}{\sqrt{\sum_{j=0}^i (g_j^{(1)})^2 + \epsilon}} g_i^{(1)},$$

where ϵ is a very small number just to prevent dividing by zero. We’ve defined the convenient notation of $\Delta\varphi$, which becomes the subject of modification for the methods hereafter. For n parameters, we denote g_i as the vector of all gradients $[g_i^{(1)}, \dots, g_i^{(n)}]$. Then, if we treat all the operations as *elementwise*, i.e. as one may expect with `numpy` arrays, we can write this again more compactly for all parameters φ as

$$\varphi_{i+1} = \varphi_i + \Delta\varphi_i; \quad \Delta\varphi_i = -\frac{\alpha}{\sqrt{\sum_{j=0}^i g_j^2 + \epsilon}} g_i.$$

One of the main reasons for the appeal in Adagrad is that you don’t really need to tune the scalar learning rate α from its initial value, since it’s being done on-the-fly for each parameter. However, an issue arises in that the sum $\sum_{j=0}^i g_j^2$ is one of positive numbers, and shall grow without bound, which will eventually reduce the learning rate to a crawl and stop learning altogether. Avoiding this is the groundwork for our next optimizers: Adadelta and RMSProp.

4.3.3 Adadelta/RMSProp

As mentioned, tackling the growing sum of squared gradients is the purpose behind Adadelta (Zeiler 2012) and RMSProp (Hinton 2018), where we'll start with the former.

Instead of maintaining a sum over the gradients g_i^2 up to step i , we recursively define a *decaying average* $E[g^2]_i$:

$$E[g^2]_i = \gamma E[g^2]_{i-1} + (1 - \gamma)g_i^2 ,$$

where we proportionally weight the previous average and the current squared gradient, each by a factor of γ and $1 - \gamma$ respectively. This is a similar idea to momentum: we're “remembering” the previous steps in some manner that we can tune numerically through γ . This leads to a $\Delta\varphi_i$ of

$$\Delta\varphi_i = -\frac{\alpha}{\sqrt{E[g^2]_i + \epsilon}} g_i . \quad (4.3)$$

Coincidentally, this is actually the equation for the *RMSProp* update, developed independently from Adadelta around the same time! For Adadelta though, we're not quite done yet though; the Adadelta authors noted that this update of $\Delta\varphi_i$ – just like the update in *any* of the methods above – does not have the same units as the parameters (it's instead dimensionless), which is not in principle an issue, but maybe better behaviour could be had by updating by a quantity of the same scale as the parameters themselves. This led to defining a second decaying average using the definition of Equation 4.3 for $\Delta\varphi_i$, which we'll also define recursively:

$$E[\Delta\varphi^2]_i = \gamma E[\Delta\varphi^2]_{i-1} + (1 - \gamma)\Delta\varphi_i^2 .$$

This expression is then also put under a square root with the same small ϵ , and we use this in place of the static learning rate α , i.e. replace it with $\sqrt{E[\Delta\varphi^2]_i + \epsilon}$. At least, we'd like to – this would lead to some kind of nested recursion relation between $E[\Delta\varphi^2]_i$ and $\Delta\varphi_i$, so we need to instead need to approximate this with a value we have access to. The paper does this with the value from the previous iteration: $E[\Delta\varphi^2]_{i-1}$. This at last gives us the full relation for one Adadelta update:

$$\Delta\varphi_i = -\frac{\sqrt{E[\Delta\varphi^2]_{i-1} + \epsilon}}{\sqrt{E[g^2]_i + \epsilon}} g_i . \quad (4.4)$$

A curious thing to note in Equation 4.4 is the lack of α – we've removed the scalar learning rate altogether, and instead only need to specify the decay factor γ before undergoing optimization.

4.3.4 Adam

We've reached **Adam** (Kingma and Ba 2014): by far the most common default choice of optimizer for deep learning, and the one frequently used within this thesis. Adam draws upon ideas from all of the above methods; it keeps track of both a decaying average of gradients *and* squared gradients. We can write their forms explicitly:

$$\begin{aligned} m_i &= \beta_1 m_{i-1} + (1 - \beta_1) g_i \\ v_i &= \beta_2 v_{i-1} + (1 - \beta_2) g_i^2 , \end{aligned}$$

where we've introduced separate decay factors β_1 and β_2 for each quantity. If you remember earlier, we were using $E[g]_i$ notation for these types of quantities, and that's not a coincidence – they're moving averages, and so are Monte Carlo estimations of expectation values (albeit off by decay terms etc). Specifically, m_i and v_i are estimators of the first moment (mean) and second moment (variance) of the gradients g_i , hence their variable names, and the name of Adam (adaptive *moment* estimation).

One thing the Adam authors note is the fact that they used the algorithm through initializing m_i and v_i as vectors of zeroes, and then found that the resulting estimates of the gradient moments were biased towards zero. The paper includes a brief derivation of the actual value of these moments, and shows that in either case of m_i or v_i , you can correct for this bias by dividing through by $(1 - \beta^i)$, where we explicitly raise β to the power of the iteration number i (the paper uses t instead). This results in the bias-corrected version of the previous formula:

$$\begin{aligned} \hat{m}_i &= \frac{m_i}{1 - \beta_1^i} \\ \hat{v}_i &= \frac{v_i}{1 - \beta_2^i} . \end{aligned}$$

We then use these bias-corrected moment estimates to construct an expression for the Adam update, which looks a lot like that for RMSProp in Equation 4.3:

$$\Delta\varphi_i = -\frac{\alpha}{\sqrt{\hat{v}_i} + \epsilon} \hat{m}_i .$$

As you can see, gradient descent can get pretty complicated! The reason I went through this explicitly was to show that gradient descent has been extremely well-studied during the rise of deep learning, and we often need to go beyond simple update rules in order to effectively learn the properties we want from our parameters in practice. In fact, the main work you'll see in the first application later on initially wouldn't learn at all until we switched to using Adam!

5 Automatic differentiation

(Hamilton et al. 2013), (Alwall et al. 2011), (Hunter 2007)

One may think that the pace of scientific discovery is determined by the speed at which new ideas are formed. That was likely true in the early days; if I posited that a rock, when thrown, will roughly trace a parabolic arc, we likely don't need to take leaps in experimental physics to test this hypothesis to some ballpark degree of accuracy – maybe we could even get away with just a ruler and the naked eye. In contrast to this, science as done in the present requires a little additional technology in order to probe the questions that we're interested in (unless we get really, really good rulers).

I say this to emphasize that the advancements made in deep learning over the past couple decades can be largely attributed to the ability to run *efficient and exact* learning algorithms at scale. For this, we have **automatic differentiation** to thank (which we playfully term “autodiff”), which allows us to take the gradient of pretty much arbitrary computer code. Which is pretty damn cool.

This section will take a tour through the basics of gradient computation, and then we'll compare the different types of automatic differentiation mechanisms (do we build a graph of our program before executing the code, or do we trace it at runtime?), and then show some example code for each.

5.1 Building blocks of automatic differentiation

The core idea of autodiff is the breaking down of a potentially complicated calculation into a set of computational **primitives**: basic operations with known derivatives. Think of things like $+$, \times , $-$, \div , \sin , \log , and so on. We know how to take the derivative across each of these operations analytically, so we can say to a computer “Every time you see a \sin , replace it with a \cos in the gradient calculation”. Then, thanks to the chain rule, we can build up the gradient of the whole program by multiplying these gradient results together.

Getting into the specifics of this, we'll begin by focusing on a function $F : \mathbb{R}^n \rightarrow \mathbb{R}$, which is a scalar valued function that takes in a vector input of dimensionality n , and returns a scalar. We deliberately choose this to mimic an objective function as seen in deep learning, which typically maps a high-dimensional vector of weights & biases to a single real number. We can also explicitly denote the application and output of F as $F(\mathbf{x} \in \mathbb{R}^n) \rightarrow y \in \mathbb{R}$.

If we break down F into a composition of (arbitrarily) four other functions, we would write that as $F = D \circ C \circ B \circ A$. Each one of these can be any random operation, like adding 5, taking the logarithm, or hooking into your OS to gain `root` access (equivalent to the identity operation from a numerical perspective). We can write this explicit chain of computations as $y = F(\mathbf{x}) = D(C(B(A(\mathbf{x}))))$, where we can interpret the computation as starting from the inner level, i.e. application of A to \mathbf{x} , then B to $\mathbf{a} =$ the output of $A(\mathbf{x})$, and so on. Let's also define $\mathbf{b} = B(\mathbf{a})$, $\mathbf{c} = C(\mathbf{b})$, and $y = D(\mathbf{c})$.

We'll see why function composition is important to cover – a core idea of automatic differentiation is to break down the gradient of the whole into the composition of the gradient of its parts via the chain rule. But more on that later.

Let's turn to gradients: we define the **Jacobian matrix** of partial derivatives of F as

$$J_F(\mathbf{x}) = F'(\mathbf{x}) = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}, \quad (5.1)$$

assuming y has multiple components (y_1, y_2 , etc.). However, since we're going from $\mathbb{R}^n \rightarrow \mathbb{R}$, the Jacobian is just one row vector:

$$F'(\mathbf{x}) = \left[\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \dots, \frac{\partial y}{\partial x_n} \right].$$

Given the decomposition of F above, we can break this down into a product of individual Jacobian matrices for each of the intermediate functions via the chain rule:

$$F'(\mathbf{x}) = \frac{\partial y}{\partial \mathbf{c}} \frac{\partial \mathbf{c}}{\partial \mathbf{b}} \frac{\partial \mathbf{b}}{\partial \mathbf{a}} \frac{\partial \mathbf{a}}{\partial \mathbf{x}},$$

One can note the sizes of each of the intermediate matrices in the format (# rows, # columns):

$$\begin{aligned} \text{size}(\partial y / \partial \mathbf{c}) &= (1, \text{len}(c)) \\ \text{size}(\partial \mathbf{c} / \partial \mathbf{b}) &= (\text{len}(c), \text{len}(b)) \\ \text{size}(\partial \mathbf{b} / \partial \mathbf{a}) &= (\text{len}(b), \text{len}(a)) \\ \text{size}(\partial \mathbf{a} / \partial \mathbf{x}) &= (\text{len}(a), n) \end{aligned}$$

The size of the final Jacobian matrix is then $(1, n)$, as shown earlier (i.e. one row vector). We'll come back to why these sizes are important – for instance, these matrices could be very hard to store if n is large.

This kind of sequential matrix multiplication can be called “accumulating” the Jacobian piece-by-piece. The order of the multiplication of these matrixies (i.e. where to put the parentheses) matters to optimize computational load, but we’ll look at two particular extreme cases:

- **Forward accumulation:** Start from the input and work forwards to the output (right to left)

$$F'(\mathbf{x}) = \frac{\partial y}{\partial \mathbf{c}} \left(\frac{\partial \mathbf{c}}{\partial \mathbf{b}} \left(\frac{\partial \mathbf{b}}{\partial \mathbf{a}} \cdot \frac{\partial \mathbf{a}}{\partial \mathbf{x}} \right) \right),$$

Here’s an example of what that first matrix product looks like:

$$\frac{\partial \mathbf{b}}{\partial \mathbf{a}} \cdot \frac{\partial \mathbf{a}}{\partial \mathbf{x}} = \frac{\partial \mathbf{b}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial b_1}{\partial x_1} & \cdots & \frac{\partial b_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial b_m}{\partial x_1} & \cdots & \frac{\partial b_m}{\partial x_n} \end{bmatrix}.$$

- **Reverse accumulation:** vice-versa!

$$F'(\mathbf{x}) = \left(\left(\frac{\partial y}{\partial \mathbf{c}} \cdot \frac{\partial \mathbf{c}}{\partial \mathbf{b}} \right) \frac{\partial \mathbf{b}}{\partial \mathbf{a}} \right) \frac{\partial \mathbf{a}}{\partial \mathbf{x}},$$

Again, let’s take a look at the result of the first matrix product:

$$\frac{\partial y}{\partial \mathbf{c}} \cdot \frac{\partial \mathbf{c}}{\partial \mathbf{b}} = \frac{\partial y}{\partial \mathbf{b}} = \left[\frac{\partial y}{\partial b_1}, \frac{\partial y}{\partial b_2}, \dots, \frac{\partial y}{\partial b_n} \right]$$

Why is that so much smaller than forward accumulation? Our initial matrix $\partial y / \partial \mathbf{c}$ has only one row due to y being 1-dimensional. Moreover, we note that this causes the size of every intermediate matrix product to always be $(1, \dots)$, meaning if we have this situation where we’re going from $\mathbb{R}^n \rightarrow \mathbb{R}$ like with F , reverse accumulation looks much more efficient in terms of memory usage and compute to get the same result, since we’re only ever storing intermediate vectors and not high-dimensional matrixies. This is the typical setting with a neural network: we have a very large input space (could even be ~billions of parameters), and we want to evaluate the Jacobian matrix of a scalar (which would have one row and ~billions of columns) with respect to those parameters. If we had the complementary setting, i.e. $\mathbb{R} \rightarrow \mathbb{R}^n$, which could maybe be some parametrization of a simulator that produces high-dimensional data, we would probably want to compute the Jacobian with forward-mode accumulation instead.

5.1.1 Jacobian-vector/vector-Jacobian products

Let's touch again on this idea of only storing intermediate vectors: we can see this arose in the case of reverse accumulation from the fact that our first multiplication had a 1 in the external dimensions, i.e. was a *row* vector \mathbf{v}^T multiplying from the left. We can recover this situation for forward mode if we pre-multiply the Jacobian matrix by some *column* vector \mathbf{v} from the right. This leads us to think about the generality offered by considering Jacobian-vector and vector-Jacobian products (JVP/VJPs) as primary functions of forward and reverse mode autodiff respectively.

To illustrate this with equations, we can write a JVP for our function F with the same operation ordering as with the *forward* accumulation of a Jacobian:

$$F'(\mathbf{x}) \mathbf{v} = \frac{\partial y}{\partial \mathbf{c}} \left(\frac{\partial \mathbf{c}}{\partial \mathbf{b}} \left(\frac{\partial \mathbf{b}}{\partial \mathbf{a}} \left(\frac{\partial \mathbf{a}}{\partial \mathbf{x}} \mathbf{v} \right) \right) \right)$$

Thinking of the rules of matrix multiplication, we note that $\frac{\partial \mathbf{a}}{\partial \mathbf{x}} \mathbf{v}$ is only tractable if \mathbf{v} is of size $(n, 1)$, since $\frac{\partial \mathbf{a}}{\partial \mathbf{x}}$ is of size $(\text{len}(\mathbf{a}), n)$. Provided this is the case, all following computations will include 1 as one of the outer dimensions, meaning we once again only need to consider intermediary vectors instead of matrices when computing this quantity.

Now, you may be thinking “Nathan, this is all well and good, but what *is* the vector \mathbf{v} , and why are you showing it to me? Aren't we interested in the Jacobian itself, and not its product with some arbitrary vector?”

Firstly, I would respond by asking why you're saying this in a thick British accent. After that, I would then go on to say that we can still use this formulation to recover the whole Jacobian – we can simply let \mathbf{v} be a *one-hot encoding* (or *unit vector* if you're more mathematically inclined) of one of the input dimensions, e.g. $\mathbf{v} = [1, 0, \dots, 0]^T$, and the result of our JVP will then be the first *column* of the Jacobian:

$$F'(\mathbf{x}) \mathbf{v} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} \\ \frac{\partial y_2}{\partial x_1} \\ \vdots \end{bmatrix} \tag{5.2}$$

We can repeat this for each dimension by changing the place we put the 1 in \mathbf{v} , then concatenate the results to get the whole Jacobian. So by building up the Jacobian one column at a time when doing forward accumulation, we gain this advantage we talked about earlier of only storing intermediate vectors, and never having to instantiate any potentially large matrices, regardless of the dimensionality of the input or output.

Ah, but wait a minute, I used y_1, y_2 etc. above – my mistake, we don't actually have a vector for our choice of F from earlier. We only have just one scalar output y . That means that the

result of our computation above would be the single first element of the Jacobian: $\partial y / \partial x_1$, and we would need one JVP calculation for each element. That seems a bit excessive! Wasn't reverse mode meant to be better? Shouldn't we use that?

Agreed. Let's do the same thing, and produce a *vector-Jacobian product* with a one-hot encoding of the output dimensions.

$$\mathbf{v}^T F'(\mathbf{x}) = \left(\left(\left(\mathbf{v}^T \frac{\partial y}{\partial \mathbf{c}} \right) \frac{\partial \mathbf{c}}{\partial \mathbf{b}} \right) \frac{\partial \mathbf{b}}{\partial \mathbf{a}} \right) \frac{\partial \mathbf{a}}{\partial \mathbf{x}} \quad (5.3)$$

$$= \left[\frac{\partial y_1}{\partial x_1}, \frac{\partial y_1}{\partial x_2}, \dots, \frac{\partial y_1}{\partial x_n} \right]. \quad (5.4)$$

We've calculated the first *row* of the Jacobian, and can construct the full thing with a VJP for each row, corresponding to each dimension of the output. In the case of this output y being scalar as before, that would make $\mathbf{v}^T = 1$ (only one output dimension), and we recover the full Jacobian in one go, since it was only one row to begin with! But of course, if y had multiple dimensions (say 5), we would only have to compute 5 VJPs to form the whole Jacobian, never having to worry about the size of the intermediate quantities.

Based on these appealing properties, it helps when using autodiff to consider the JVP/VJP as the fundamental operation when calculating gradients of programs in practice. It's a funny way of thinking at first, but the quantity we end up with is just the regular Jacobian (or elements thereof) in the end, so it's only important when considering implementation details of gradient computations.

To summarize: we've seen the difference between **forward-** and **reverse-mode** autodiff, and their usefulness in constructing Jacobians via **Jacobian-vector** and **vector-Jacobian products**, which bypass the need to store large intermediate matrices by forming the Jacobian one column or one row at a time respectively. We also note that for the deep learning case of interest, where we have an objective function F that maps $\mathbb{R}^n \rightarrow \mathbb{R}$ with n large, we far prefer *reverse-mode* autodiff to calculate its gradient, which we need to perform optimization.

5.1.2 From sequences to graphs

One thing that you may have noticed in our previous section is the fact that we focused only on a simple decomposition of F into the sequential application of four functions A , B , C , and D to the input \mathbf{x} . In reality, computer programs are going to look a lot more complicated, and will be represented by the more general construct of a directed acyclic graph (DAG). We need to adapt the above framework for JVPs/VJPs in order to generalize to these real-life scenarios.

It turns out this is fairly simple: we only need to consider two additional cases than what we've considered already. The application of a single operation with a single input and output would

be represented as one node in a graph, with an edge going in and coming out. Luckily, the only additional generalization we need to consider is the case of multiple inputs (fan-in) and multiple outputs (fan-out).

For the fan-in case, i.e. multiple input values from different computations: we know how to calculate Jacobians for a single input, so we can just do this process for each input separately. More explicitly: for $F(\mathbf{a}, \mathbf{b})$, with \mathbf{a} and \mathbf{b} possibly coming from different parts of the program, we calculate the Jacobian for each input separately as before: $F'_{\mathbf{a}}(\mathbf{a}, \mathbf{b}) = \partial y / \partial \mathbf{a}$ and $F'_{\mathbf{b}}(\mathbf{a}, \mathbf{b}) = \partial y / \partial \mathbf{b}$.

Fan-out is slightly more involved, since we now have the case of multiple return values. Let's examine a function with this behaviour: $G(\mathbf{x}) = [3\mathbf{x}, 5\mathbf{x}]^T$. We can see that this input replicates our input \mathbf{x} with different factors applied to each output, which we can represent through the linear function $G(\mathbf{x}) = [3I, 5I]^T \mathbf{x}$, where I is the identity matrix. The Jacobian of G is then just the coefficients multiplying \mathbf{x} : $G'(\mathbf{x}) = [3I, 5I]^T$. But in practice, we're probably going to be computing a VJP across this node in the graph during backpropagation. Remembering that this involves multiplying by a vector \mathbf{v}^T with the same dimensionality of the output of G , we can then write $\mathbf{v}^T = [\mathbf{v}_1^T, \mathbf{v}_2^T]$, one vector for each vector in $G(\mathbf{x})$. This then leads to

$$\mathbf{v}^T G'(\mathbf{x}) = [\mathbf{v}_1^T, \mathbf{v}_2^T] [3I, 5I]^T \quad (5.5)$$

$$= 3\mathbf{v}_1^T + 5\mathbf{v}_2^T. \quad (5.6)$$

So if we have a function with multiple outputs, we'll be accumulating the VJP of that function across the outputs through addition. We can see that this results from the shapes of the vectors being multiplied here, which will always result in an outer shape of $(1, 1)$, so we can safely generalize this to any number of outputs.

That's pretty much all the scaffolding we need in terms of a framework to calculate gradients. The only missing pieces are:

- A way to express the program in a graph
- An implementation of the vector-Jacobian and Jacobian-vector operations

We'll discuss both of these in the following sections.

5.2 Building the computation graph

There are two main existing strategies to represent a series of code computations as a graph. One involves letting the user build up the graph structure manually via library-provided primitives – called **define-and-run**; the resulting construct is known as a *static graph*, and is the approach taken by libraries like [Theano](#) and [TensorFlow](#) (when run without eager execution). This has

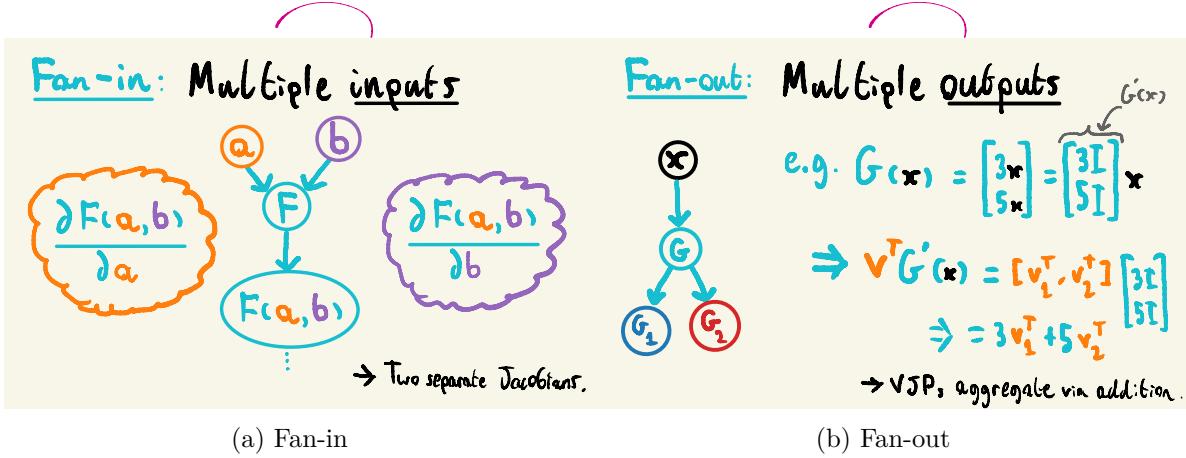


Figure 5.1: Demonstration of how functions that fan-in and fan-out are handled when gradients are computed with respect to their input(s).

the unfortunate side effect of making code much more difficult to read and write, since you have to use symbolic proxies for operations like control flow and looping (e.g. `tf.while_loop` instead of Python's `while`) in order to instantiate that operation in the graph.

The other approach, known as **define-by-run**, builds up a *dynamic graph* structure during a program's execution. How does this work? The program is *traced* at runtime, meaning that the autodiff framework is watching which operations occur when a function is run in order to build up the computation graph for that function. When done this way, incorporating loops and conditional structure within the graph is no longer needed: at runtime, loops are unrolled into sequences, and the branching induced by conditional logic will collapse to one branch when the program is actually ran. These properties make define-by-run the more popular approach to autodiff, and is the approach taken by libraries such as **JAX**, **PyTorch**, and **Tensorflow (eager execution mode)**. It's worth noting that since evaluating the gradients requires tracing the program, i.e. evaluating the function, the runtime cost for the gradient calculation is usually of the same order as the program itself. Why? For each primitive in the program, there's a corresponding step in the gradient computation (e.g. wherever you see a $\log x$ in your program, there'll be a $1/x$ somewhere in the JVP/VJP call), so the computations are almost totally identical in compute¹.

5.3 Differentiating fixed points

We spend a bit of time here on the more niche topic of differentiating a fixed point, as we make use of this result later. A **fixed point** x^* of a function f is defined by the relation

¹This may not hold when you're doing fancy things like checkpointing, which I haven't covered here.

$$f(x^*) = x^*,$$

meaning if we apply f (even multiple times), we remain stationary at the point we applied f to. Why is this of interest, i.e. what kind of functions of importance exhibit this behavior?

The first and easiest thing is of course the straight line $f(x) = x$, which has the whole real line as fixed points. But maybe we're more interested in the case where the fixed point is a quantity of interest – this is the case for something like an *optimization loop*. Here's an example where f is one gradient descent step:

$$f(x, \text{loss}) = x - \frac{\partial \text{loss}}{\partial x} (\times \text{learning rate etc.}) \quad (5.7)$$

$$\Rightarrow f(x^*, \text{loss}) = x^*; \quad x^* = \operatorname{argmin}_x \text{loss}. \quad (5.8)$$

As above, if our gradient descent is any good, then we'll hopefully converge to the fixed point x^* , which is the value of x that lies in some local minimum of the loss function. Further iterations will then not do anything – we'll still be sitting at x^* . How might we take the gradient of this fixed point? Moreover, what if this gradient is with respect to parameters that implicitly define the loss itself?

The first thing to highlight is that in practice, we'd take many steps to reach the minimum, which corresponds to many sequential applications of f to some initial value of x . In the framework of automatic differentiation outlined in previous sections, this would mean taking the gradient (in a define-by-run setting) would *unroll* the optimization loop at runtime, and decompose *each* of these per-iteration applications of f into their primitives, and compose their vector-Jacobian products or similar. For an optimization loop, this could involve thousands of steps! Moreover, all that work that happens in the early stages of optimization far from the fixed point x^* will likely not impact the gradient of the fixed point itself – we're much more interested in the steps close to convergence.

To get around this computational issue, we can employ the use of the **implicit function theorem**. The full details of the theorem are beyond the scope of this application, but it guarantees some things that we'll state here. To be consistent with later sections, we will now switch symbols from x to θ (which will denote parameters we're optimizing), and include φ as parameters that *implicitly* define part of f (e.g. that define the objective function used in optimization). Now, for a different function $g(\theta, \varphi)$, where there exists some solution $g(\theta_0, \varphi_0) = 0$, then the following holds:

A *solution mapping function* exists in the form of $\theta^*(\varphi)$ such that

- $\theta^*(\varphi_0) = \theta_0$
- $g(\theta^*(\varphi), \varphi) = 0 \quad \forall \varphi$

- θ^* is *differentiable* with respect to φ !

To put this into words: as long as there exists *some* solution that makes $g(\theta, \varphi) = 0$, we get a mapping for the *general solution* as a function of φ , which is differentiable. This means that as long as we find a way to calculate that gradient, we can directly access the gradients of the solution θ_0 that we found during optimization with respect to the particular φ_0 that we used, all thanks to the general function θ^* .

Now, notice that we wrote this holding for $g(\theta, \varphi) = 0$, which we don't have quite yet. But we can define this for our update state f by simply letting $g(\theta, \varphi) = f(\theta, \varphi) - \theta$. Now, when we arrive at our solution θ_0 as the fixed point of f for some φ_0 , we'll get $g(\theta_0, \varphi_0) = \theta_0 - \theta_0 = 0$, and in turn have access to all those nice properties! We just need to explicitly calculate the gradient of θ^* now, which we can do by differentiating both sides of $g(\theta^*(\varphi), \varphi) = 0$:

$$\frac{\partial g(\theta^*(\varphi), \varphi)}{\partial \varphi} = \frac{\partial g}{\partial \theta^*} \frac{\partial \theta^*}{\partial \varphi} + \frac{\partial g}{\partial \varphi} .$$

Then in practice, we'll have θ_0 as our optimization solution and φ_0 as our implicit parameters, which we can plug in, and then rearrange for $\partial \hat{\theta} / \partial \varphi$:

$$\frac{\partial \theta^*}{\partial \varphi} = \frac{\partial \theta_0}{\partial \varphi_0} = - \left[\frac{\partial g}{\partial \theta_0} \right]^{-1} \frac{\partial g}{\partial \varphi_0} .$$

Finally, we can substitute in our definition of g in terms of f to get

$$\frac{\partial \theta_0}{\partial \varphi_0} = \left[I - \frac{\partial f}{\partial \theta_0} \right]^{-1} \frac{\partial f}{\partial \varphi_0} .$$

We've constructed an expression for the gradient of the fixed point θ_0 of an update rule f , and with respect to the parameters φ that define the objective used in the optimization! This is a fantastic result, as it means we can just use this expression instead of unrolling the entire optimization loop itself, saving us lots of memory and compute in the process.

To read more about this construction, and some of the finer details of the implementation on the autodiff side (note how we skipped over the conversation about the fact that we have VJPs and not gradients directly), I would thoroughly recommend (Duvenaud, Johnson, and Kolter, n.d.), which I based this section upon.

5.4 Other approaches to taking gradients of programs

I've given most of the spotlight of this section to automatic differentiation, since it's the best existing way to differentiate programs, and it makes up part of the core of my applications of machine learning to physics in later sections. However, there are a number of alternative ways to calculate gradients that we'll briefly study now in order to give some perspective on the landscape of existing methods.

5.4.1 Numerical differentiation

I wouldn't be surprised if one of the first things you thought before reading this section is that we can approximate the gradient of a function at x pretty handily already by just evaluating it at both x and a point close by $x + \Delta x$, then computing

$$\frac{\partial f}{\partial x} \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$

We can see how well this performs on an example problem in Figure 5.2 for different step sizes, and in Figure 5.3 for different numbers of evaluations. A smaller Δx will result in higher accuracy for that point, but if we're interested in the actual gradient function, this will then incur many evaluations of the function itself (twice for each gradient estimate) as we build up the envelope of the gradient, or use it frequently in a program (e.g. gradient descent). Moreover, if we want higher-order derivatives, then the error induced in the estimate of $\partial f / \partial x$ from the step size Δx not being identically 0 will compound upon finite difference estimation of $\partial^2 f / \partial x^2$ and so on.

5.4.2 Symbolic differentiation

Symbolic differentiation endeavors to calculate gradients through algebraic symbols, just like doing it on pen and paper. This approach will definitely appeal at first sight to those that have done any kind of calculus – if we want to differentiate a function that implements $y = x^2$, then we will instantly think of $2x$, not of Jacobian-vector products or the like. In this sense, the gradients of the functions produced are analytical. However, even for a simple program, these expressions can swell easily to become horrifically complex compared to the resulting programs from autodiff.

We'll omit any further discussion for now for the sake of brevity, but for a much more thorough comparison between this and other methods compared to automatic differentiation, I'll direct your attention to the nicely-written notebook here that I looked at for inspiration while writing this whole section: (Heinrich 2020).

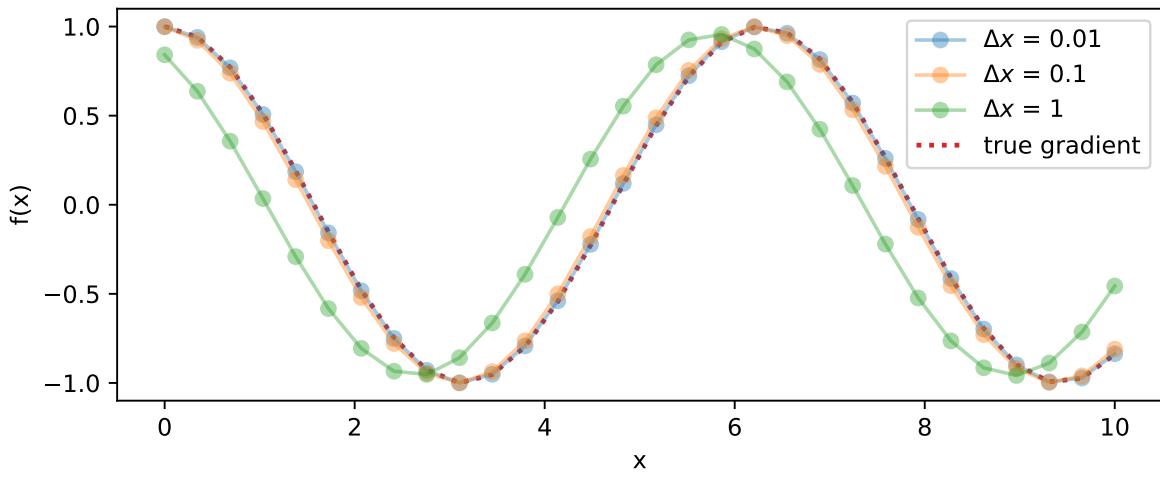


Figure 5.2: Finite difference gradient calculations for the function $y=\sin(x)$, varying the distance between the evaluated points.

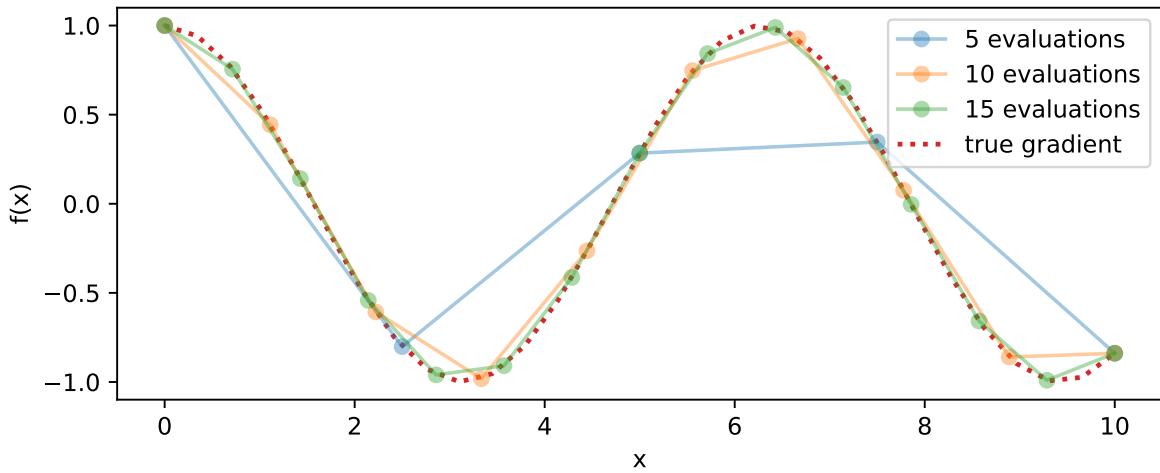


Figure 5.3: As in Figure 5.2, but varying the number of gradient evaluations with a fixed step size of $1e-4$.

6 Machine learning

The blanket term **machine learning** indicates a shift in mindset for how computers complete a given task. When presented with such a task, one may try to solve it through a pen and paper worked conceptual solution. It is then up to us to tell the computer – in excruciating detail in its own language – each of the individual steps needed to implement the solution we came up with. This is known as *programming* a computer. But what if there was a way to show the computer many examples of our problem, and use an algorithm to *learn* a good solution by updating some internal state?

That's machine learning! We find some inspiration for this in a quote from the fantastically written essay in (Samuel 1962), which is stated in the context of comparing human-written programs to possibly learned ones:

There are many mental processes that people are called upon to perform that cannot be, or at least have not been, reduced to a simple set of rules. Take the process of playing a game of chess, not of simply adhering to the rules of the game, but rather the process of playing a good game against an intelligent opponent. There are no known procedures for guaranteeing a win, and yet people learn to play the game and some few become very proficient. – Arthur L. Samuel

The basic idea (also made reference to in that essay) is this: maintain some internal state – literally just a set of numbers, which could e.g. pick a pre-defined strategy based on a value – and then update that internal state in some way by checking the performance. This rather simple statement carries a lot of ambiguous ideas, such as

- a notion of internal state
- some way to combine that state with data to produce a result
- a performance metric to assess the result after applying the state
- an update rule to improve the value of the state based on the performance

These ideas form the cornerstone of machine learning approaches, and we'll unpack them all in detail below. Before continuing though, it's worth noting the distinction between *machine* learning and *deep* learning – the latter is a subset of the former, and refers to a particular paradigm involving complex neural networks. Machine learning makes no assumptions on the form of the machine itself.

Machine learning methods follow a shared set of abstract steps: given a dataset, we

- define a **model** with **parameters** φ (where the model is a way to combine φ with the data)
- construct a measure of performance for the model, called the **objective function**
- **fit** the model to the dataset through some update rule
- use the *learned* model to perform **inference** (apply the model to new data)

We can see this workflow reflected in the API of modern software packages, such as **scikit-learn** (Buitinck et al. 2013) and **keras** (Chollet et al. 2015). Using this framework and terminology, we’ll explore some useful models, reflecting on the developments that have occurred as a by-product of the modern era of computing.

6.1 Neural networks and deep learning

A model that would certainly be useful is one that can model the solution to any task at all. **Neural networks** are indeed this class of model; inspired by the way the brain handles the processing of information, they are proven to be *universal approximators*, i.e. given a *continuous function* $g(\mathbf{x})$, where \mathbf{x} is an arbitrary-length vector of real-valued inputs, there exists a value of parameters φ such that a neural network $f(\mathbf{x}, \varphi)$ satisfies

$$|g(\mathbf{x}) - f(\mathbf{x}, \varphi)| < \epsilon \quad \forall \mathbf{x}, \text{ for } \epsilon > 0 . \quad (6.1)$$

This is great! Though, it’s not necessarily this property that makes neural networks so popular, it’s more the fact that we can practically attain this performance. Said another way, it’s not just that there exists φ , but that we can often find it in real life! This can be attributed both to the effectiveness of *gradient descent* as a learning algorithm, and the software/hardware that we have access to that breathes life into the training process.

So: what *is* a neural network in the first place?

At its simplest, a neural network is a sequence of location-scale transforms of the input data, with non-linear “activation” functions applied in-between to allow for non-linear modelling capabilities. This type of neural network is referred to as a **multi-layer perceptron** (MLP) or a **feed-forward network** (both namings given since I use them interchangeably in later sections). Each layer of an MLP represents a round of these computations. At its most complex, there’s a lot of funky ways to transform the data, including self-attention, convolutions, graph structure, and all sorts of other stuff. These types of specialized “architectures” are beyond the scope of what we’ll look at here, but are incredibly important for introducing inductive bias that helps to more efficiently identify useful information within the data.

The ingredients to a MLP are the **weights** w , the **biases** b , and the **activation functions** σ . The weights represent the scale transform, and the bias the location transform. On the other hand, the activation function plays the role of “bending” the output such that we can model non-linear effects, i.e. anything with realistic complexity. Examples of common activation

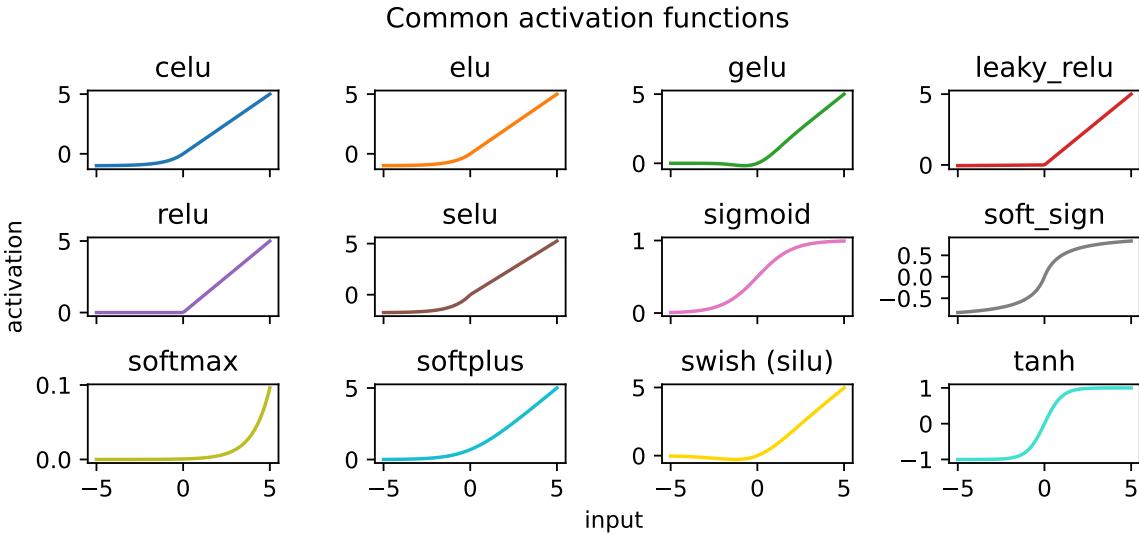


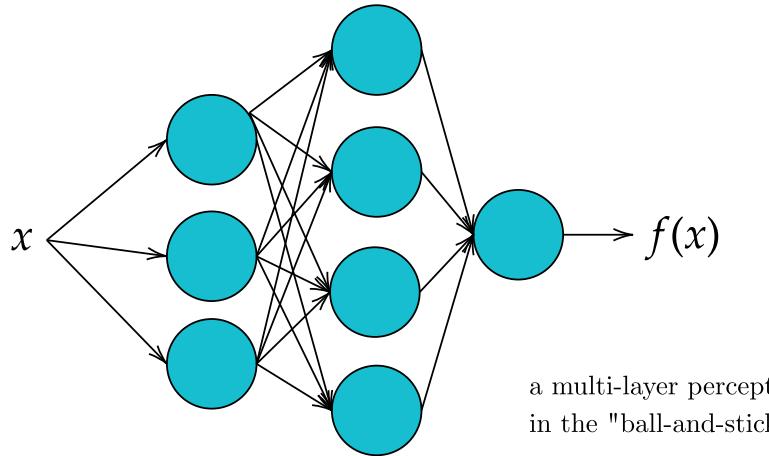
Figure 6.1: Commonly used activation functions, taken from the Python library JAX.

functions can be found in Figure 6.1, where there are all sorts of flavors to choose from, each with their own quirks (ReLU and its variants have been the gold standard for some time).

You'll typically see all this represented in a ball-and-stick diagram, e.g. Figure 6.2. Each series of balls represents one set of computations with the weights, biases, and activation functions that are within that layer. The outputs from this are called activations (just to reference the application of the activation function). The thing we call a **layer** is then each set of parallel computations of this nature, which are then aggregated into the set of inputs to the next layer (if it exists, else it's just the network output). Don't get too hung up on this definition of the word "layer" though, it sort of breaks down when looking at modern architectures with very detailed computation steps.

6.1.1 What's a “layer” in a MLP?

Here's a compact formula for a computation of a single layer. Given a set of n activations from the previous layer (0th layer meaning just the data points), and k neurons in layer i , the output of applying the neurons to the activations to obtain the $i + 1$ th layer is represented as a matrix equation:



a multi-layer perceptron (MLP),
in the "ball-and-stick" representation

Figure 6.2: The “ball-and-stick” representation of a MLP.

$$\underbrace{\begin{bmatrix} a_0^{(i)} \\ a_1^{(i)} \\ \vdots \\ a_n^{(i)} \end{bmatrix}}_{\text{activations for layer } i+1} = \sigma \left(\underbrace{\begin{bmatrix} w_{0,0} & w_{0,1} & \cdots & w_{0,n} \\ w_{1,0} & w_{1,1} & \cdots & w_{1,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{k,0} & w_{k,1} & \cdots & w_{k,n} \end{bmatrix}}_{\text{weight matrix}} \underbrace{\begin{bmatrix} a_0^{(i)} \\ a_1^{(i)} \\ \vdots \\ a_n^{(i)} \end{bmatrix}}_{\text{activations for layer } i} + \underbrace{\begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{bmatrix}}_{\text{bias vector}} \right)$$

$$\Rightarrow \mathbf{a}^{(i+1)} = \sigma(\mathbf{W}\mathbf{a}^{(i)} + \mathbf{b}) ,$$

where applying the activation σ is distributed to its elements, i.e.

$$\sigma \left(\begin{bmatrix} x \\ y \\ z \end{bmatrix} \right) = \begin{bmatrix} \sigma(x) \\ \sigma(y) \\ \sigma(z) \end{bmatrix} . \quad (6.2)$$

This is essentially the definition of a neuron (the ball in the ball-and-stick diagram shown in Figure 6.2): a neuron is the j th function in a layer i that maps the activations $\mathbf{a}^{(i)}$ from the previous layer into the j th element of the $i + 1$ th activation vector $\mathbf{a}^{(i+1)}$, with a functional form as indicated in Equation 6.2. The sticks in that diagram would represent the elements of the weight matrix \mathbf{W} , with missing connections between neurons a and b corresponding to zeroing out the $w_{a,b}$ term in the weight matrix.

If we put the weights and biases for each layer all into one vector of parameters, that's what we've been calling φ , which represents the entire internal state of a neural network. If we then bottle up the way we apply φ to the data within the function f – whether that be as simple as the MLP above or something more complex – we can compactly represent a neural network as $f(\mathbf{x}, \varphi)$ as above in Equation 6.1.

Since a neural network is a sequence of applications of Equation 6.2, it's differentiable with respect to the parameters φ (and even if it's more complex, this differentiability is always made to be present). That means we can optimize our neural network with **gradient descent**, which we spent considerable time on in the previous section.

One extra thing to mention is the different type of architectures that go beyond this simple MLP framing. We can think about these architectures as a kind of inductive bias on the space of possible functions that could be learned, e.g. through some kind of specific manipulations that take advantage of the format of the input data (sequences, images, sets etc.). To highlight a few:

- **Convolutional neural networks** (Krizhevsky, Sutskever, and Hinton 2012) are one of the first types of domain-specific architecture, and manipulate an image through convolutional filters that measure local image features through things like pooling.
- **Transformers** (Vaswani et al. 2017) perform fantastically well for sequential data (e.g. natural language), but have even shown generalization to other domains like images (Dosovitskiy et al. 2020). They use a mechanism called *self-attention* to extract information from sequential inputs, and are probably the most important architecture that exists at the time of writing in terms of their ability to generalize and scale.
- **Deep sets** (Zaheer et al. 2017) is a method that incorporates the bias of the input data being an unordered collection. They have found use in e.g. particle physics (Komiske, Metodiev, and Thaler 2019), where objects like jets and their properties exist in unequal amounts across events, but without any specific ordering (though we've typically ordered them by p_T and then treated them as a sequence in the past).
- **Geometric deep learning** (Bronstein et al. 2021) generalizes a lot of the above, and casts things in the language of equivariances and graphs, spawning the idea of e.g. graph neural networks (Scarselli et al. 2009).

There are countless other architectures, but we will focus on a particular neural network method (not necessarily an architecture) in the next section, as it makes up one of my applications, so we'll spend a bit of extra time to sufficiently ground that work.

6.2 Normalizing flows

A **normalizing flow** is a trainable density estimator based on neural networks that admits both sampling and a tractable likelihood. Flows model a vector $\mathbf{x} \in \mathbb{R}^D$ from an underlying distribution $p_X(\mathbf{x})$ as a transformation $\mathbf{x} = T(\mathbf{u})$, where $\mathbf{u} \in \mathbb{R}^D$ is a vector of samples drawn from a chosen distribution $p_U(\mathbf{u})$. We refer to the data distribution $p_X(\mathbf{x})$ as the **target distribution** that we're trying to model, and to $p_U(\mathbf{u})$ as the **base distribution** that we transform to do this. This base distribution is normally something simple like a normal distribution, which offers some guarantees as to making the flow a universal density approximator (details in Papamakarios et al. (2019)).

How does this work? The transform T is the key, and is the thing we'll be training in practice. We start by pointing out the defining property of flows, which is the requirement that T is both

- *differentiable* (the Jacobian of the transformation $J_T(\mathbf{u}) \in \mathbb{R}^{D \times D}$ exists, where $J_T(\mathbf{u})$ is defined as in Equation 5.1)
- *invertible* (the inverse transformation $T^{-1}(\mathbf{x})$ exists).
 - $T^{-1}(\mathbf{x})$ is also required to be differentiable for flows!

Given these properties, we can invoke the change of variables formula from X to U , which relates the target and base distributions by the determinant of the Jacobian matrix:

$$p_X(\mathbf{x}) = p_U(\mathbf{u}) |\det J_T(\mathbf{u})|^{-1}.$$

Here, \mathbf{u} is calculated as the inverse transformation $\mathbf{u} = T^{-1}(\mathbf{x})$ since we want the exact \mathbf{u} for our particular \mathbf{x} when evaluating the likelihood. We've also exploited the fact that the determinant of the inverse of a matrix is the inverse of the determinant.

You may have noted our extra requirement that the inverse transform is also differentiable — the existence of the Jacobian $J_{T^{-1}}(\mathbf{x})$ lets us write the change of variables above in terms of only T^{-1} and \mathbf{x} :

$$p_X(\mathbf{x}) = p_U(T^{-1}(\mathbf{x})) |\det J_{T^{-1}}(\mathbf{x})|. \quad (6.3)$$

These equations form the basis for constructing a flow, where we implement the transform T by using a neural network to control its parameters (e.g. a location-scale transform, where the location and scale are provided by a network).

One advantage of having a differentiable and invertible T is that we can compose multiple transforms in a row, with the result itself being both differentiable and invertible. Specifically, we can write, for $T = T_1 \circ T_2$:

$$T^{-1} = (T_1 \circ T_2)^{-1} = T_2^{-1} \circ T_1^{-1},$$

$$\det J_T(\mathbf{u}) = \det J_{T_1 \circ T_2}(\mathbf{u}) = \det J_{T_2}(T_1(\mathbf{u})) \det J_{T_1}(\mathbf{u}).$$

Knowing that we can stack transformations freely, we have a similar paradigm to neural networks, where stacking more “layers” (here, transforms) could bring about a more expressive model. This is the “flow” part of a normalizing flow: a series of samples from p_U are flowing through a series of transforms T to arrive at something like the target density p_X . The “normalizing” part comes from going the other direction via T^{-1} , where data samples are “normalized” back to the base distribution¹.

There are many types of transforms one can choose to satisfy these requirements (which can be partitioned into a bijective “transformer” and a non-bijective “conditioner”), but I’ll omit everything but the one I used in Section 6.2.2, and direct you to (Papamakarios et al. 2019) for a much more comprehensive review.

6.2.1 Training a flow

The goal is clear: we want to make our base distribution look like the target distribution. How do we quantify this?

Recall from Section 2.2.2 that we have a way to measure the divergence between two probability distributions through the expected difference in log-likelihood under the true distribution (or approximate distribution, noting the asymmetric result depending on our choice). Denoting the predicted distribution from the flow as $q_X(\mathbf{x}; \theta)$ (where θ comprises both the parameters of the base density γ and the parameters of the transform ϕ), and the target density as $p_X(\mathbf{x})$, we can write this explicitly as

$$D_{\text{KL}}[p_X(\mathbf{x}) || q_X(\mathbf{x}; \theta)] = -\mathbb{E}_{p_X(\mathbf{x})} [\log q_X(\mathbf{x}; \theta)] + \text{constant}$$

$$\Rightarrow -\mathbb{E}_{p_X} \left[\log p_U(T^{-1}(\mathbf{x}; \phi); \gamma) + \log |\det J_{T^{-1}}(\mathbf{x}; \phi)| \right] + \text{constant},$$

where we’ve substituted our expression for the flow likelihood in Equation 6.3.

This is a quantity we’d like to minimize, as to make p_X and q_X as “close” as possible. In practice, we’re likely going to have to substitute the expectation over the true (unknown) distribution with a Monte Carlo estimate using our data samples $x_{i=1}^N$, which turns this equation into

$$D_{\text{KL}}[p_X(\mathbf{x}) || q_X(\mathbf{x}; \theta)] \approx -\frac{1}{N} \sum_{i=1}^N \log p_u \left(T^{-1}(\mathbf{x}_i; \phi); \gamma \right) + \log |\det J_{T^{-1}}(\mathbf{x}_i; \phi)| + \text{constant}.$$

¹The naming is a bit extra, I know. But at least it’s not another play on “attention is all you need”.

This comes out to effectively minimizing the negative log-likelihood of the flow model on the data samples – we’re just fitting the model with maximum likelihood, as defined in Section 2.3.1! This is one example of how we can train a flow – we minimize this objective with respect to parameters θ , by e.g. gradient descent, since this is a differentiable expression in θ .

6.2.2 Masked Autoregressive Flows

A specific type of flow that we’ll encounter in the wild later is the **masked autoregressive flow** (Papamakarios, Pavlakou, and Murray 2017). The approach that this flow takes to density modelling is as follows:

When modelling a distribution across multiple random variables, one can break down their joint density into a product of conditional distributions through the probability chain rule as in Equation 2.3, and models these conditional distributions explicitly:

$$\begin{aligned} p(x_1, \dots, x_N) &= p(x_1)p(x_2|x_1)p(x_3|x_2, x_1)\dots p(x_N|x_{N-1}, \dots, x_1) \\ &= \prod_{i=1}^N p(x_i|\mathbf{x}_{j < i}) \end{aligned}$$

Here, we’ve arbitrarily labelled our random variables x_i with indicies i from 1 to N , and use these to construct our conditional distributions. Note, however, that we could shuffle the order of our random variables, then reassign them the index of their place in the array, and the relation would still hold. Despite this, the only important thing is that each conditional distribution assigned to x_i depends *only* on those x_j for which $j < i$, *regardless of the initial variable ordering*. This is known as the **autoregressive property**.

One can model this relationship using a neural network in a *single forward pass*. By constructing a feed-forward network with equal input and output dimensionality, and assigning the same ordering to the input and output, we can simply drop (or **mask**) those connections for each output i with all input variables that have index $j < i$. This way, there is no possible computational path between each output and the variables that come before that output in the ordering, meaning that the value of that output will be able to capture the nature of the relevant conditional $p(x_i|\mathbf{x}_{j < i})$. These aspects together form a **masked, autoregressive** network.

This idea was first used in (Germain et al. 2015), which used it to output the density directly in one forward pass by having the outputs correspond to the individual conditional distributions. However, to use this network in a flow, which transforms one distribution to another, we can instead use the outputs of the neural network to parametrize the transform T . The result is known as a **masked autoregressive flow** (MAF), and was introduced in (Papamakarios, Pavlakou, and Murray 2017).

The MAF as I used it involved a fairly simple implementation of T – a location scale transform:

$$T(\mathbf{u}; \alpha, \beta) = \alpha \cdot \mathbf{u} + \beta ,$$

where α, β are the scale and location parameter vectors respectively. These are *vectors* because there's one entry corresponding to each entry in \mathbf{u} , where the individual parameters α_i, β_i are coming from the i th output of a neural network (or more precisely, the i th pair of outputs, since we have two values α_i, β_i for every one input u_i), which has parameters itself ϕ . Training the flow is then done as in Section 6.2.1, with the masking mechanism from earlier in this section being put in place.

As a bonus, there's a simple way to condition this transform on side information \mathbf{y} that provides context: we can just add \mathbf{y} as an extra input to the network (or multiple inputs if there's more than one variable), and have it mix with every input, since each conditional distribution would also include \mathbf{y} . We then have a MAF that can perform **conditional density estimation**, i.e. estimate $p(x_1, \dots, x_N | \mathbf{y})$.

Part II

Applications

7 Data Analysis in High-Energy Physics as a Differentiable Program

This is the title track of this thesis, and rightly so; it dominated metrics in both my time spent and headspace given for any of the topics I've written about. I feel incredibly privileged to have worked on something like this, which is fairly self-contained, and draws upon themes from both machine learning and statistical inference in order to make headway in addressing a long-standing issue: *systematic-aware optimization*. What's even cooler is that it goes further than this, opening up a whole variety of possibilities to optimize with the whole statistical inference procedure in the loop, and rethink the ways in which we can improve our workflows. I hope you enjoy it!

7.1 Motivation

Given the success of the Standard Model, analysis of data from the LHC usually occurs for two reasons:

- Precisely measuring Standard Model processes to look for small deviations from their predicted values
- Searching for new physics signatures as predicted by models beyond the Standard Model

When analyzing data in this way, we'll have lots of free parameters to tune. These can be as simple as a threshold value that you limit the p_T to, or as complicated as the weights and biases that determine a neural network for identifying b -jets. We can of course choose any values for these quantities to do our analysis, but the resulting physics that follows may suffer as a result. As such, we're likely to try some kind of optimization to improve the answers to our physics questions. How do we do this in practice?

In either case above, there is a notion of signal (what you're looking for) and background (everything else). Generally, we then try to choose a parameter configuration that can separate (or discriminate) the signal from the background, allowing us to extract just the data we think is relevant to the physics process we're looking at. As an example, machine learning models are often trained using the **binary cross-entropy** loss as an objective, which corresponds to optimizing the ability of the model to identify whether an event originated from signal or background processes. A closely related goal is the **Asimov significance** in the case of signal

and background event counts s and b with *no uncertainty* on either quantity. The formula for this stems from assuming a Poisson likelihood function as in Section 3.2, and is equal to

$$Z_A = \sqrt{2 \sum_{i \in bins} ((s_i + b_i)(\log(1 + s_i/b_i)) - s_i)} . \quad (7.1)$$

As indicated in the sum, these counts can be spread across different bins in the case where your data is a histogram, but the formula is more commonly reduced to the 1-bin scenario that just deals with the overall numbers of signal and background events. In this case, we can then Taylor expand the logarithm to get

$$Z_A = \sqrt{2((s + b)(s/b + \mathcal{O}(s/b) - s))} \approx s/\sqrt{b} \quad \text{for } s \ll b.$$

This makes it much clearer to see that optimizing with respect to Z_A is just a fancier way of trying to increase the amount of signal compared to the amount of background, which is directly analogous to separating signal from background, just as binary cross-entropy would do.

Now, this is all very sensible of course (we want to discover our signal), but this approach has some shortcomings that distance the efficacy of the resulting configuration from our physics goals. A recent review of deep learning in LHC physics (Guest, Cranmer, and Whiteson 2018) lets us in on why:

(...) tools are often optimized for performance on a particular task that is **several steps removed from the ultimate physical goal** of searching for a new particle or testing a new physical theory.

(...) sensitivity to high-level physics questions **must account for systematic uncertainties**, which involve a nonlinear trade-off between the typical machine learning performance metrics and the systematic uncertainty estimates.

This is the crux of the issue: we're not accounting for uncertainty. Our data analysis process comes with many sources of systematic error, which we endeavour to model in the likelihood function as nuisance parameters. However, optimizing with respect to any of the above quantities isn't going to be aware of that process. We need something better.

Okay, I hear you: blah blah this is all just talk... let's prove this scenario needs addressing with an example!

7.1.1 A simplified analysis example, both with and without uncertainty

Let's define an analysis with a predicted number of signal and background events (e.g. from simulation), with some uncertainty on the background estimate. We'll abstract the analysis configuration into a single parameter ϕ like so:

$$s = 15 + \phi$$

$$b = 45 - 2\phi$$

$$\sigma_b = 0.5 + 0.1\phi^2$$

Note that $s \propto \phi$ and $\propto -2\phi$, so increasing ϕ corresponds to increasing the signal/background ratio. However, our uncertainty scales like ϕ^2 , so we're also going to compromise in our certainty of the background count as we do that. This kind of tradeoff between s/b ratio and uncertainty is important for the discovery of a new signal, so it may be that can't get away with optimizing s/b alone, as the p -value may be worse!

Let's start by visualizing the model itself, which we do for three values of ϕ as an example in Figure 7.1.

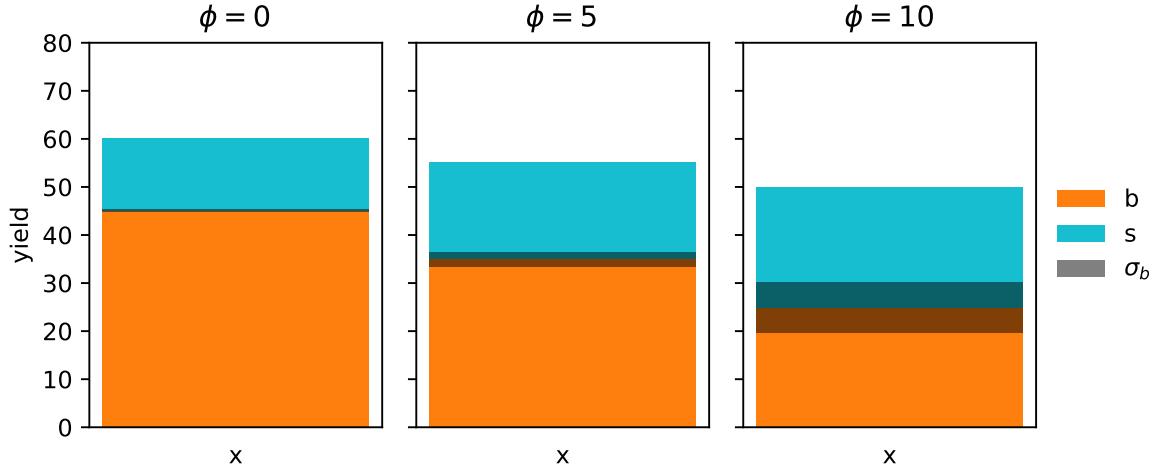


Figure 7.1: Plot of the predicted counts from our model at three values of ϕ .

Using this very simple histogram, we can form a statistical model as if we're using Section 3.2 principles, which would look something like

$$p(x|\mu) = \text{Poisson}(x|\mu x^{\text{sig}} + \gamma x^{\text{bkg}}) \text{Normal}(y|\gamma, 1) , \quad (7.2)$$

where γ is a continuous description of σ_b that we get from interpolating between the yields, just like in the HistFactory approach, which has the constraint term $\text{Normal}(y|\gamma, 1)$ attached to penalize fitting a value of γ that differs largely from the information provided by σ_b .

Using this likelihood, we can calculate the expected discovery p -value by doing a hypothesis test using the observed data as the Asimov dataset for the nominal model $\mu, \gamma = 1$. We can plot this across all the values of ϕ , and see what value gives us the lowest p -value (in practice, scanning over the space is computationally impossible for a given analysis configuration and a complicated model). We do this in Figure 7.2, where we include the result using a model both with and without uncertainty. Notice how much the curves differ; if we optimized the model without uncertainty (i.e. optimize for signal/background separation only), we'd end up at the *worst* solution! This is pathologically constructed of course, but it goes to show that these objectives don't talk to each other directly.

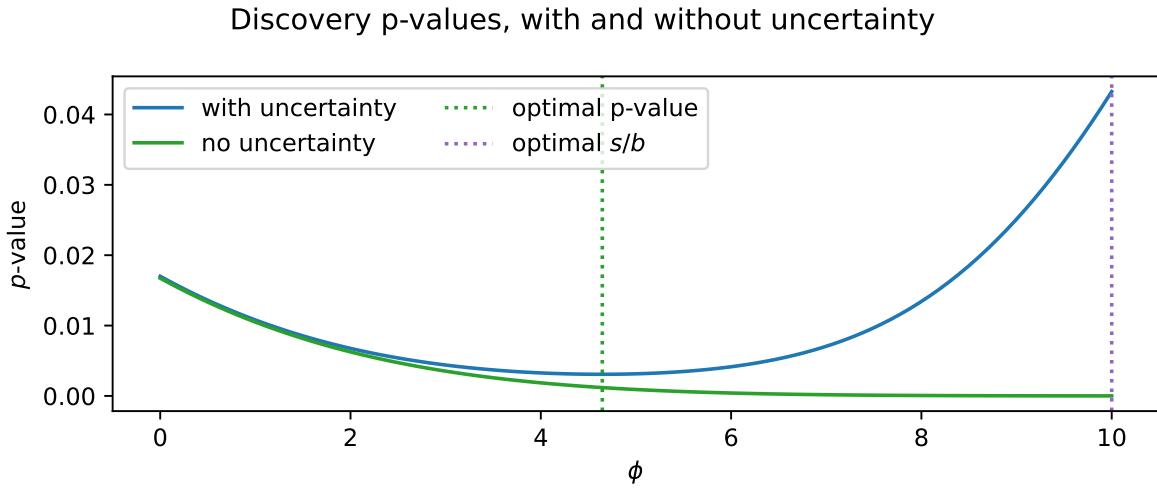


Figure 7.2: Plot of the calculated p -value from using our statistical model across of ϕ , both including the uncertainty and neglecting it.

If we optimize this analysis then, we want to arrive at the value of ϕ at the dotted green line (around ~ 4.3 or so), which gives us the benefit of rejecting the background hypothesis more strongly when the signal exists in the data. This is made possible if we use the p -value as our objective – it clearly accounts for the uncertainty!

The reason for this makes sense: in these physics likelihoods, we're careful to include all the details of the systematic uncertainties that we're able to quantify by constructing nuisance parameters that vary the shape and normalization of the model. From here, to calculate the p -value, we then construct the **profile likelihood ratio** as a test statistic, which accounts for these systematic uncertainties by fitting the value of the nuisance parameters depending on the hypothesis you test (see Section 2.3.3 for more).

All this makes the p -value seem like a good candidate for an objective function! So why haven't we used this already?

As emphasized in Chapter 4, if we want to perform optimization using gradient-based methods,¹ then we need the objective that we optimize to be *differentiable*. This is not immediately the case for the p -value – we would have to be able to differentiate through all stages of the full calculation, including model building, profiling, and even histograms, which are not generally known for their smoothness. But say we were able to decompose this complicated pipeline into bite-size chunks, each of which we can find a way to take gradients of. What becomes possible then? This begins our view of **data analysis in high-energy physics as a differentiable program**.

In the following sections, we'll take a collider physics analysis apart step-by-step, then see how we can employ tricks and substitutes to recover gradients for each piece. After that, we'll explore the ways that we can use the result to perform gradient-based optimization of different parts of the analysis with respect to physics goals. We'll then do it all at once by *optimizing a toy physics analysis from end-to-end*, exploring the common example of a summary statistic based on a neural network, accounting for uncertainties all the while.

7.2 Making HEP Analysis Differentiable

The goal of this section is to study components within a HEP analysis chain that are not typically differentiable, and show that when we overcome this, we can employ the use of gradient-based optimization methods – both to optimize free parameters jointly, and to use objectives we care about. From there, we'll examine the typical steps needed to calculate the sensitivity of a physics analysis, and see how we can make that whole chain differentiable at once, opening up a way to incorporate the full inference procedure when finding the best analysis configuration.

First, we're going to jump right in with an example to illustrate how we can take advantage of gradient descent to optimize a typical problem faced in collider physics analyses: choosing the best selection criteria.

7.2.1 A simple example: cut optimization with gradient descent

We begin with a toy signal and background distribution over some variable x , where the signal lies as a peak on top of an exponentially decaying background, as shown in Figure 7.3.

A quintessential operation for data filtering in HEP is the simple threshold, also called a **cut**: we keep all data above (or below) a certain value of the quantity we're concerned with. To

¹We don't have to use gradient based methods! They're just very well implemented and studied, as well as enabling things like this paradigm.

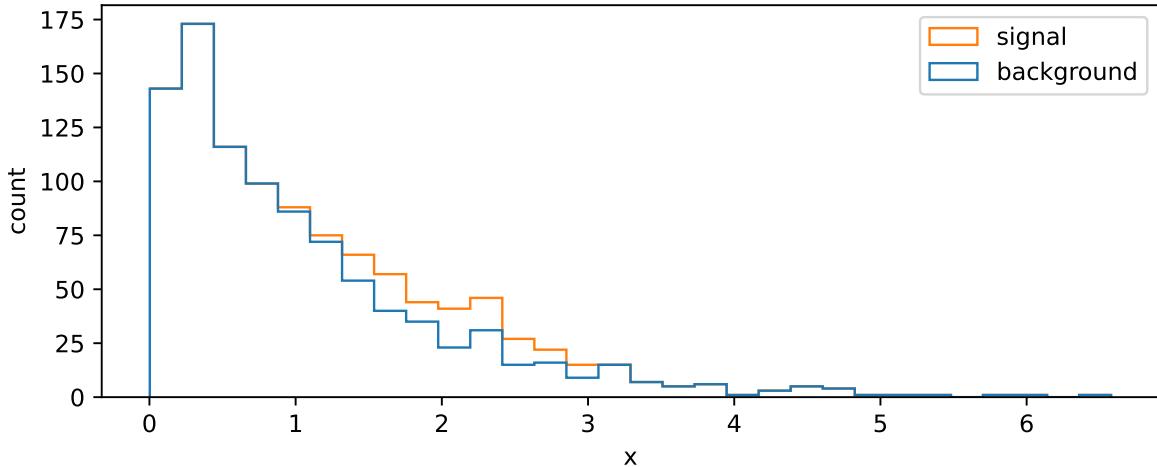


Figure 7.3: Histogram of a situation with a simple exponentially falling background and a small signal peak.

increase the significance (e.g. as defined by Equation 7.1), we can try to remove data such that we increase the overall ratio of signal to background. In Figure 7.3, it looks like there's not much signal for low values of x , which motivates us to put a cut at say $x = 1$. We can see the result of applying this cut in Figure 7.4, where we've increased the Asimov significance compared to using no cut at all.

We had a nice go at a guess, but how do we pick the *best* cut? For this simple problem, it suffices to scan over the different significances we'll get by cutting at each value of x , then just use the value with the highest significance. Doing this leads to the optimal cut being around $x = 1.54$. In reality, though, this could be an expensive procedure to do for a wide range of x and for many different cut variables. This prompts the search for some kind of intelligent optimization that can handle large dimensional parameter spaces. Gradient descent is just that! But, to make it work, we need to be able to calculate the gradient of the significance with respect to the cut value – something only possible if the cut itself is differentiable (it isn't).

To see this, note that cuts are step functions, i.e. logical less than or more than statements. These can be viewed as applying weights to the data – 0 on one side of the threshold, and 1 on the other. If we change the cut value, the events either keep their weight (0 change in significance) or sharply gain/lose their weight value (discrete jump in significance). We would then like to replace this thresholding with a *smooth* weight assignment such that the cut value varies smoothly with the weights applied. What kind of operation can do this? We have such a candidate in the *sigmoid function* $1/(1 + e^{-x})$.

Normally, the sigmoid serves as a method to map values on the real line to $[0,1]$, so we leverage this to be used as a cut by applying it to data, which results in a set of weights for each point

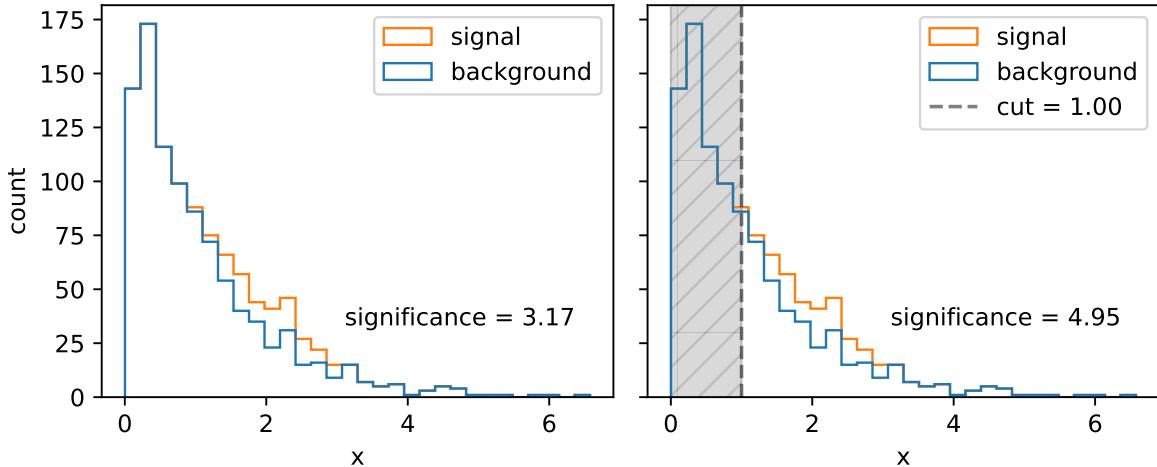


Figure 7.4: Comparing the significance resulting from applying a cut to no cut at all.

in $[0,1]$. (A normal cut does this too, but the weights are all 0 or 1, and you drop the 0s. One could similarly threshold on a minimum weight value here.)

Practically, we introduce slope and intercept terms that control the sigmoid's x position and how “hard” the cut is: $1/(1 + e^{-\text{slope}(x - \text{cut value})})$. This slope allows us to control the degree to which we approximate the cut as a thresholding operation, with higher values of the slope meaning less approximation (but this will also increase the variance of the gradients, as we’re getting closer to the discrete situation outlined previously). See the sigmoid plotted with different slopes in Figure 7.5.

Now that we have a differentiable cut, we can see what the significance scan looks like for both the differentiable and standard cases, shown in Figure 7.6. It’s an interesting plot; there’s a clear smoothing out of the overall envelope of the significance in comparison to using the hard cut. However, the important thing is the **coincidence of the maxima**: when optimizing, we’ll use the differentiable cut, but we’ll plug the value of the cut position from the optimization back in to the hard cut for our actual physics results. This is a very important distinction – *we don’t use approximate operations in the final calculation!* Moreover, since we can control the degree to which we’re approximating the significance landscape, one could even imagine a fine-tuning of the slope when we’re close to a local minima during optimization, allowing us to make jumps more in-line with the true optimum value (though this is not explored here).

Now that we’ve done the groundwork, we can do the optimization and see if we converge to the correct result! Using gradient descent and the Adam optimizer with a learning rate of $1e-3$, we find the cut shown in Figure 7.7 (we optimize $1/Z_A$ since we’re doing minimization). The significance (calculated with the *hard* cut) is extremely close to the best possible value, so I’d call this a success!

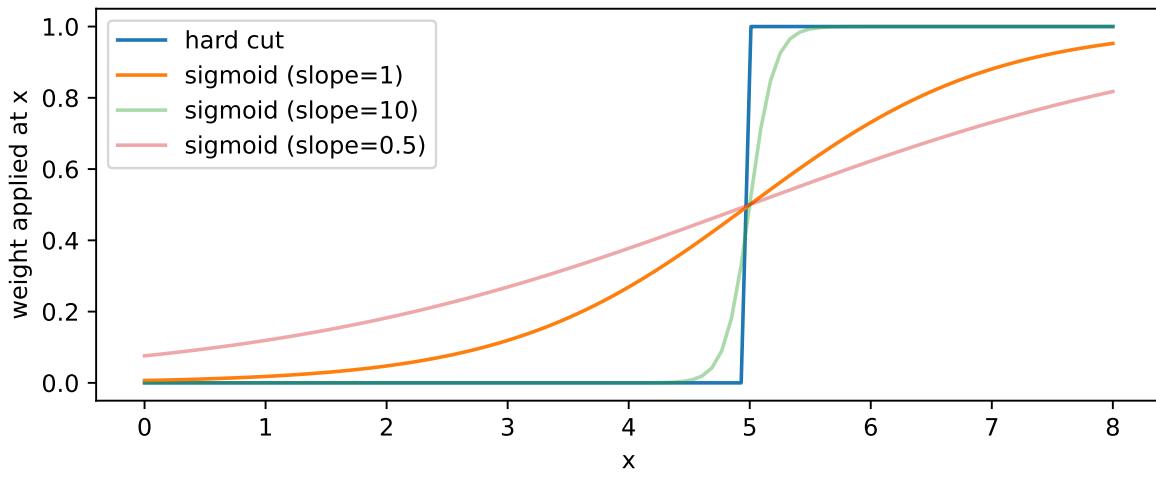


Figure 7.5: Comparing the sigmoid to a regular hard cut for different values of the sigmoid slope.

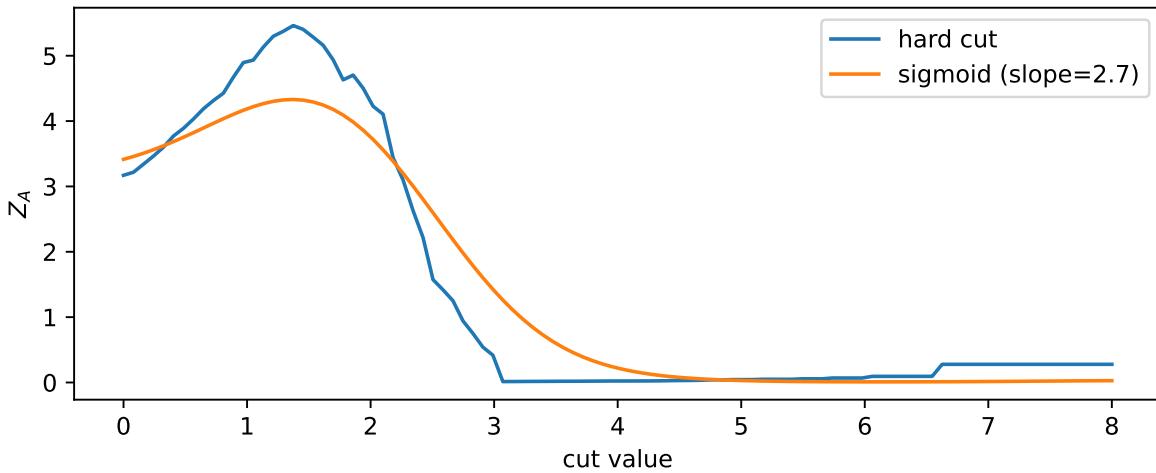


Figure 7.6: A scan over all cut values to find the best resulting Asimov significance – both for the regular cut, and for the sigmoid.

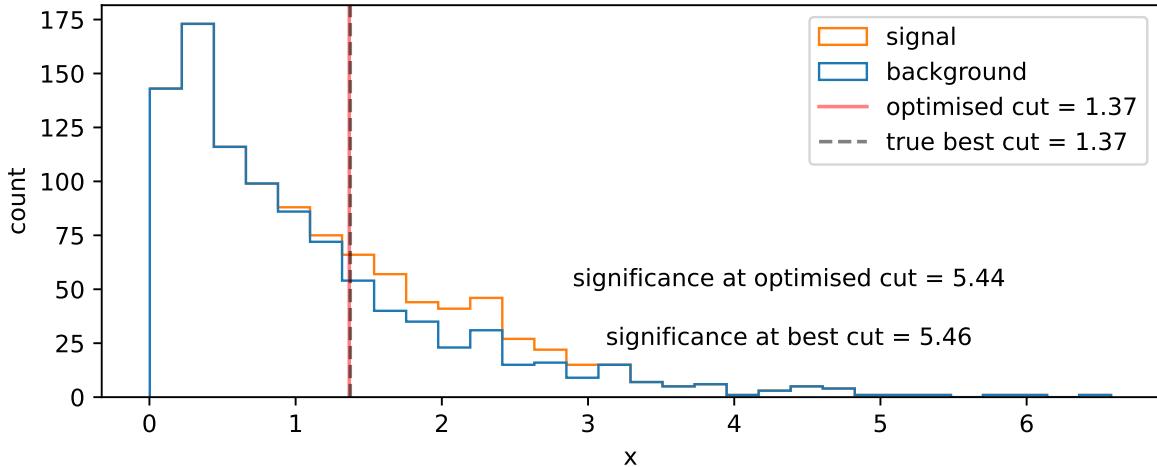


Figure 7.7: The resulting cut from optimization compared to the true best cut. Significances in both cases are shown.

7.2.2 Examining a typical analysis

Now that we've looked at an example of the kind of thing we may want to do, we can zoom out and look at the big picture. Given a pre-filtered dataset, a commonly used analysis pipeline in HEP involves the following stages:

1. Construction of a learnable 1-D summary statistic from data (with parameters φ)
2. Binning of the summary statistic, e.g. through a histogram
3. Statistical model building, using the summary statistic as a template
4. Calculation of a test statistic, used to perform a frequentist hypothesis test of signal versus background
5. A p -value (or CL_s value) resulting from that hypothesis test, used to characterize the sensitivity of the analysis

We can express this workflow as a direct function of the input dataset \mathcal{D} and observable parameters φ :

$$CL_s = f(\mathcal{D}, \varphi) = (f_{\text{sensitivity}} \circ f_{\text{test stat}} \circ f_{\text{likelihood}} \circ f_{\text{histogram}} \circ f_{\text{observable}})(\mathcal{D}, \varphi). \quad (7.3)$$

Is this going to be differentiable? To calculate $\partial CL_s / \partial \varphi$, we'll have to split this up by the chain rule into the different components, which can be written verbosely as

$$\frac{\partial \text{CL}_s}{\partial \varphi} = \frac{\partial f_{\text{sensitivity}}}{\partial f_{\text{test stat}}} \frac{\partial f_{\text{test stat}}}{\partial f_{\text{likelihood}}} \frac{\partial f_{\text{likelihood}}}{\partial f_{\text{histogram}}} \frac{\partial f_{\text{histogram}}}{\partial f_{\text{observable}}} \frac{\partial f_{\text{observable}}}{\partial \varphi}. \quad (7.4)$$

In the case of an observable that has well-defined gradients with respect to ϕ (e.g. a neural network), the last term in Equation 7.4 is possible to calculate through automatic differentiation. But none of the other terms are differentiable by default! We're going to have to figure out some way to either *relax* (make differentiable) these operations, or use tricks to make the gradient easier to calculate. This is explored in the following sections, starting with the histogram.

7.2.3 Binned density estimation (histograms)

Histograms are discontinuous by nature. They are defined for 1-D data as a set of two quantities: intervals (or *bins*) over the domain of that data, and counts of the number of data points that fall into each bin. For small changes in the underlying data distribution, bin counts will either remain static, or jump in integer intervals as data migrate between bins, both of which result in ill-defined gradients. Similarly to the cut example with the sigmoid, we're assigning a number (there the weight, and here a count in a bin) in a discrete way to the data – to make this differentiable, we need to come up with a smooth version of this that allows gradients to be calculated across the result.

To say a little more to that effect, we'll look at the types of gradients that we may be interested in. Say we have a data distribution that depends on some latent parameter μ , e.g. data that's drawn from $\text{Normal}(\mu, 1)$. We can then make a histogram of the resulting data. What happens to that histogram When we shift the value of μ ? Well, shifting the mean will just translate the histogram along the x -axis; an example of this is shown in Figure 7.8 for a couple values of μ (with the random seed kept constant).

Let us now shift our focus to a single bin: we'll choose the bin centered on 0, and monitor its height as we vary μ , shown in Figure 7.9.

We can see that the bin height jumps around in discrete intervals as we translate the underlying data, which would produce ill-defined gradient estimates if we used something numerical like finite differences. To exploit the magic of automatic differentiation here, we want to make some other function such that this envelope becomes smooth; varying μ by a very small amount should also vary the bin height by a small amount instead of leaving it static or jumping discontinuously.

The solution that we developed to address this involves a **kernel density estimate** (KDE). We discussed this in Section 3.1.2, but just to recap: a KDE is essentially the average of a set of normal distributions centered at each data point, with their width controlled by a global parameter called the **bandwidth**. There's a neat way to take this and cast it into a bin-like form (i.e. defined over intervals): We can calculate the “count” in an interval by taking the area under the KDE between the interval endpoints. We can do this using the cumulative

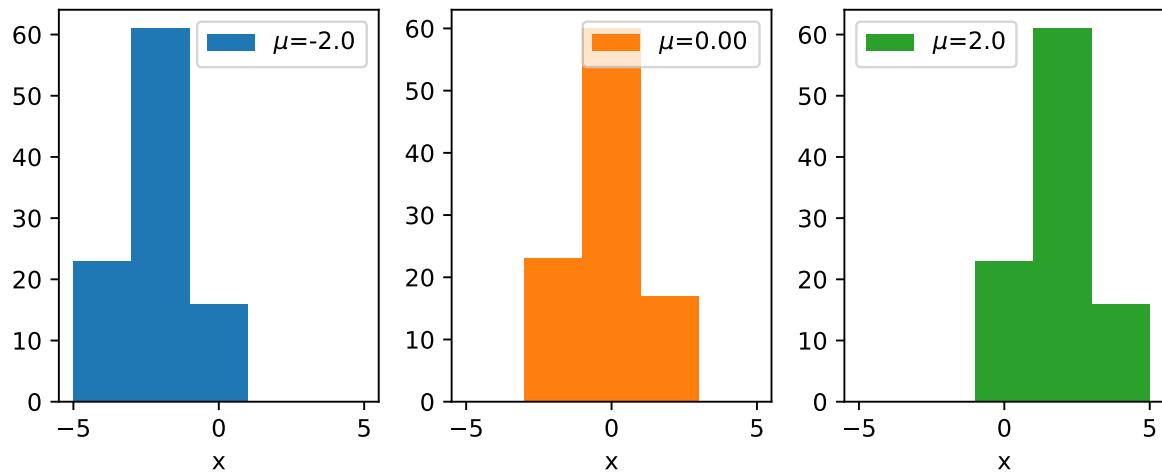


Figure 7.8: Translating a histogram from left to right by varying the center of the distribution the data is drawn from.

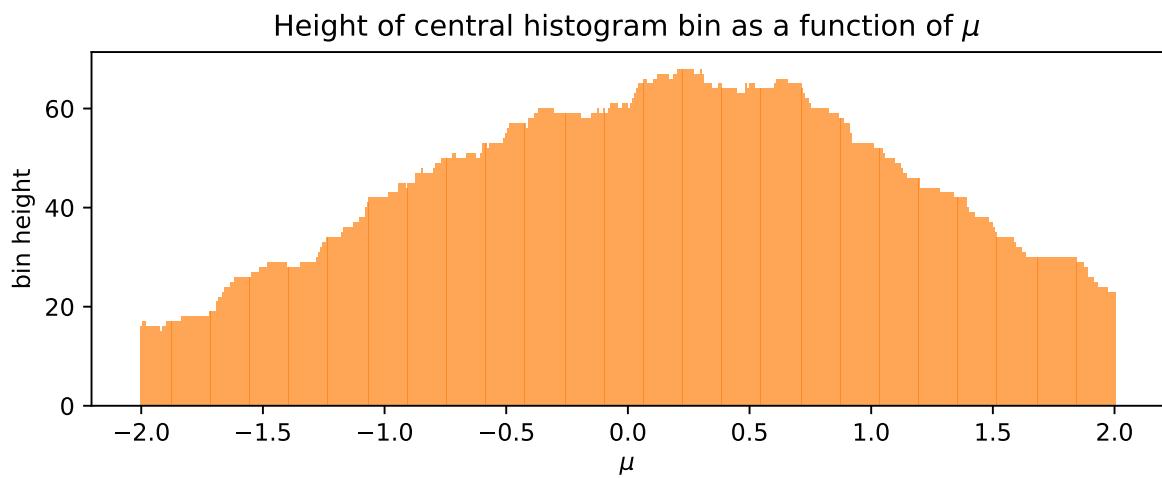


Figure 7.9: Demonstrating the shift in the central histogram bin as μ is varied from -2 to 2.

density function (cdf), as $P(a \leq X \leq b) = P(X \leq b) - P(X \leq a)$. Since the KDE is the mean over some normal distributions, its cdf is also just the mean of the cdfs for each normal distribution. Moreover, to turn this into a histogram-like object, we can multiply the result by the total number of events, which just changes the mean into a sum. We put this all together in Figure 7.10, where a pseudocoded implementation of a **binned KDE** (bKDE) can be found.

```
def bKDE(data: Array, bins: Array, bandwidth: float) -> Array:
    edge_hi = bins[1:] # ending bin edges ||<-
    edge_lo = bins[:-1] # starting bin edges -> ||
    # get cumulative counts (area under kde) for each set of bin edges
    cdf_hi = norm.cdf(edge_hi.reshape(-1, 1), loc=data, scale=bandwidth)
    cdf_lo = norm.cdf(edge_lo.reshape(-1, 1), loc=data, scale=bandwidth)
    return (cdf_hi - cdf_lo).sum(axis=1) # sum cdfs over each kernel
```

Figure 7.10: ?(caption)

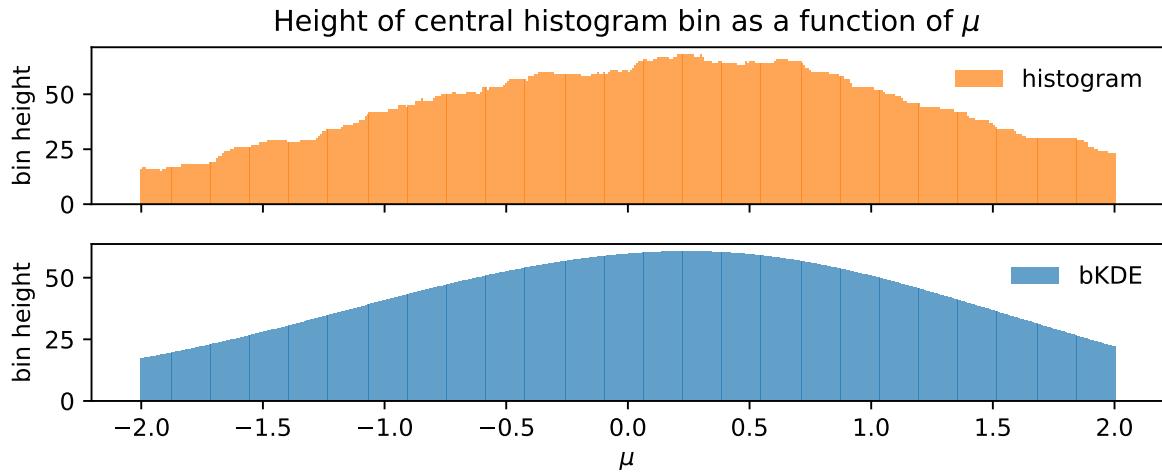


Figure 7.11: Demonstrating the shift in the central histogram bin as μ is varied from -2 to 2 for both a regular histogram and a bKDE.

Using this, we can remake the plot from Figure 7.9 for the bKDE, which we can see in **?@fig-bin-height-bKDE**, showing that the variation of the bin height with μ is much more well-behaved.

Choosing the bandwidth

I'll show a few studies here that illustrate what happens to the accuracy of the bKDE histogram from the perspective of both the distribution and the resulting gradients.

We know what happens to a KDE when we change the bandwidth: small bandwidth gives a function with high variance, and a large bandwidth oversmooths the distribution. How do these effects impact the bKDE? We can quantify this *relative to the bin width* by examining the shape of the bKDE relative to a “hard” histogram, which is shown in Figure 7.12. For low bandwidths, we recover something almost resembling a regular histogram. In fact, in the limit of zero bandwidth, we will *exactly* get a histogram! The reason is that zero bandwidth would turn each normal distribution into an infinite spike at each data point, which, when integrated over to get the counts, would have a contribution of 1 if the event lies in the bin, and 0 otherwise².

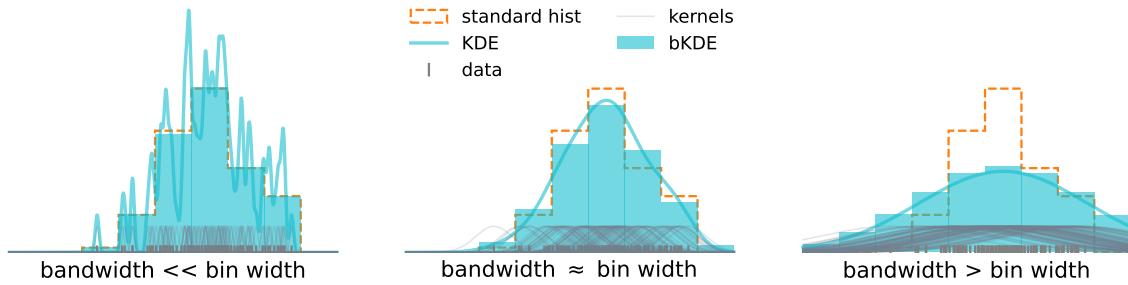


Figure 7.12: Illustration of the bias/smoothness tradeoff when tuning the bandwidth of a bKDE, defined over 200 samples from a bi-modal Gaussian mixture. All distributions are normalized to unit area. The individual kernels that make up the KDE are scaled down for visibility.

This idea of a bias/variance tradeoff with the bandwidth is the gist of it, but there’s an additional factor that will influence the value of the bandwidth chosen: the number of data samples available. We may expect that as we add more samples to a KDE, there will be a lot more kernels centered on the new points, so we’d want to reduce the bandwidth in order to faithfully represent the envelope of the distribution. We then can inspect the degree to which this also continues to hold for the bKDE; it may be that good defaults for KDEs differ slightly compared to those for bKDEs.

First, let’s examine the distribution accuracy as a function of bandwidth and number of data samples. We can define this by looking at the “true” histogram, which can be calculated using the cumulative distribution of $\text{Normal}(\mu, 1)$ in a way analogous to the bKDE (i.e. the integral under the curve over the intervals defined by the bins), which we then normalize to the number of data samples available. We can then plot the true height of the central bin as it varies with μ , and compare it to that obtained from the histogram and bKDE estimates across a number of different settings for the sample size and bandwidth. These plots are shown in

²For non-uniform bin widths, an extension of the bKDE to non-uniform bandwidths could be interesting – one could keep the bin width/bandwidth ratio fixed for each bin, and if the event falls in a given bin, the resulting bandwidth from using that ratio is applied to that event. This would make the analogy between bin width and bandwidth more general in some ways, albeit at the cost of someone’s coding time.

Figure 7.13, which looks at bandwidths of 0.05, 0.5, and 0.8 in tandem with sample sizes of 20, 100, and 5000. As expected, we see that the low bandwidth case has the histogram and bKDE predictions for the bin mostly agreeing, while they diverge for larger bandwidths. The best-case scenario appears to be when we have a large number of samples and a low bandwidth, which is when we'd expect all three estimates to converge. If we choose a bandwidth too large though, we're going to introduce a bias as we oversmooth the data features.

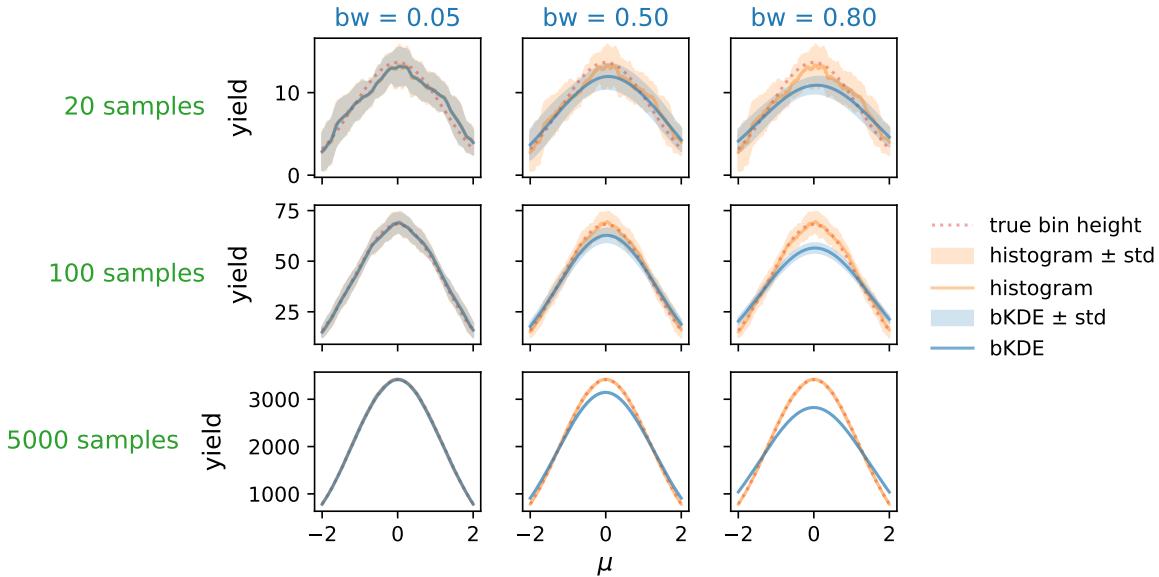


Figure 7.13: Demonstrating the shift in the central histogram bin as a function of bandwidth and the number of samples for a histogram and bKDE, which are compared to the true bin height.

So far things seem all to follow intuition somewhat, but we've only checked half the picture; the whole reason we're using the bKDE construct in the first place is so we can access *gradients* of the histogram yields. To study these, we can derive the “true” gradients from the definition of the bin height: as before, a bin defined by (a, b) for a given μ value is just

$$\text{yield}_{\text{true}}(\mu; a, b) = \Phi(b; \mu, \sigma) - \Phi(a; \mu, \sigma) ,$$

where $\Phi(x; \mu, \sigma)$ is the normal cumulative distribution parametrized by $\sigma, \mu =$. We can then just take the gradient of this expression with respect μ by hand. First we write the explicit definition of the cdf:

$$\Phi(x; \mu, \sigma) = \frac{1}{2} \left[1 + \text{erf} \left(\frac{x - \mu}{\sigma \sqrt{2}} \right) \right] ,$$

where the convenient short hand of the error function erf is given by

$$\text{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dx .$$

Then, the derivative is as follows:

$$\frac{\partial}{\partial \mu} \Phi(x; \mu, \sigma) = \frac{1}{2} \left[1 - \left(\frac{2}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \right) \right] ,$$

since $\frac{d}{dx} \text{erf}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}$.

As mentioned, we have $\sigma = 1$ in this particular example, making this expression simpler:

$$\frac{\partial}{\partial \mu} \Phi(x; \mu, \sigma = 1) = \frac{1}{2} \left[1 - \left(\frac{2}{\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2}} \right) \right] .$$

Putting this all together gives us

$$\Rightarrow \frac{\partial}{\partial \mu} \text{yield}_{\text{true}}(\mu; a, b) = -\frac{1}{\sqrt{2\pi}} \left[\left(e^{-\frac{(b-\mu)^2}{2}} \right) - \left(e^{-\frac{(a-\mu)^2}{2}} \right) \right] ,$$

which we can use as a way to quantify the accuracy of the gradients obtained from using a bKDE compared to those of the amount of the true distribution in the interval (a, b) .

The comparative plots between the true gradient, the histogram gradient, and the bKDE gradient are shown in Figure 7.14, where the histogram gradient is calculated using the finite differences method, and the bKDE gradient with automatic differentiation. A similar trend can be seen to Figure 7.13, where the estimate from the bKDE improves with more samples, and becomes much less noisy. This is in contrast to the histogram, which struggles with gradients unless the sample size is large (here 5000), and produces very high variance estimates in general. The bKDE, however, is able to avoid this high variance while keeping a reasonably low bias depending on how many samples are present; the central plot, for instance, shows a case where the bKDE of bandwidth 0.5 far outperforms estimating the true gradient with just 100 samples compared to the erratic estimates using the regular histogram.

It seems then that there is some kind of middle ground to be had with respect to the bandwidth one can choose for a bKDE depending on the number of samples present, where the trends of distribution and gradient accuracy roughly align. Optimality seems to be in the high-sample and low-bandwidth case. To look at this at scale, we can summarize each of these plots into a single number, e.g. the mean relative error, and see how this number varies across a large grid of different configurations for the number of samples and the bandwidth. This plot can be found in Figure 7.15, where a number of grid points are taken for combinations of bandwidth/sample size, and the absolute relative error in the gradient has been calculated (and averaged across

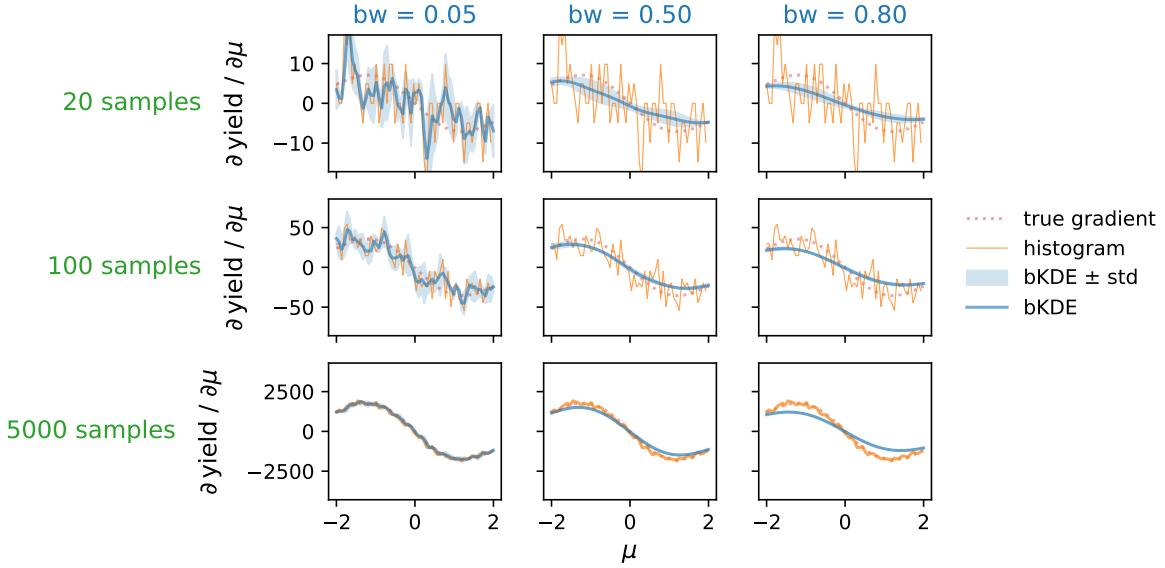


Figure 7.14: Variation of the gradient of the central histogram bin as a function of bandwidth and the number of samples for a histogram and bKDE, which are compared to the true gradient of the yield.

three random seeds, then a second averaging over 500 values of μ in (-2,2)). Orange scatter points are overlaid to show the bandwidth choice that yields the minimum relative error given each of the studied sample sizes. The trend is generally in agreement with that which we saw in Figure 7.14 of higher sample size letting us choose lower bandwidths, but there's definitely a little pause for thought given the couple points that deviate from forming a neat straight line. There also appears to be a little pocket of lower error around 2000 samples, which doesn't appear to have any obvious explanation. Given more time, one could study this in detail with a much finer grid (memory and temporal limitations prevented expanding this further), and for a variety of different examples, then maybe perform [symbolic regression](#) to infer a good rule of thumb. This could also be recasted into a rule of thumb relative to the bin width, which could be a useful metric for comparison (e.g. in Figure 7.12 shown earlier).

Other differentiable binned density estimates

In the INFERNO paper (Castro and Dorigo 2019), from which much inspiration was taken in general, they use a softmax function as a way to mimic binned output from the neural network, which would have an output dimensionality equal to the number of bins you want in your histogram. We can then think about each data point having a weight of 1, and having the softmax smoothly distribute that weight across the different bins. For a dataset \mathbf{x} and a fixed neural network \mathbf{y} with output nodes y_i up to y_N , the yield of bin i in the histogram is

Absolute relative error on the gradient across a bKDE (single-bin example)

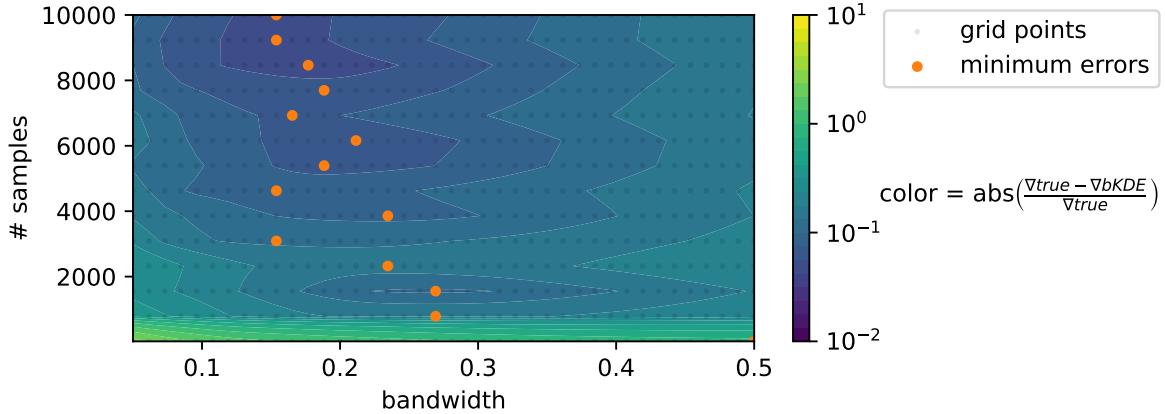


Figure 7.15: Absolute relative error in the bKDE gradient compared to the true distribution, calculated for a wide variety of bandwidths and sample sizes. Orange points indicate the lowest error across the rows of constant sample size to hint at the trend of a good bandwidth choice.

calculated by summing the softmax contributions from each data point in that bin:

$$\text{softmax histogram}_{\text{bin } i}(\mathbf{x}) = \sum_{\text{data } k} \text{softmax}(x_k, y_i) \quad (7.5)$$

$$= \sum_{\text{data } k} \frac{e^{y_i(x_k)/\tau}}{\sum_{j=0}^N e^{y_j(x_k)/\tau}}, \quad (7.6)$$

where τ is a factor to tune how hard the slope of the softmax is, i.e. it has some analogy to the bandwidth about tuning the level of approximation. A drawback, however, is that the softmax used in tandem with a neural network does not come with an inherent notion of *ordering*; it's going to be somewhat arbitrary in which bins events occupy, and the resulting plots are a little hard to interpret compared to regular histograms. Also, even the “hard” softmax with $\tau \rightarrow \infty$ is difficult to map to some other “true” histogram in which the bins follow Poisson-distributed counts.

As for other things, one could always do something like overlap sigmoid functions, or even make a KDE with a new histogram-like kernel. We'll cap our imagination here though, and move onwards to the likelihood that this histogram is part of.

7.2.4 Differentiable likelihood construction

Now, I must confess, I have told you a bit of a white lie to set up the motivation here. The likelihood function as described in Equation 3.5 is indeed a-priori differentiable with respect to the histograms that make up the expectations. The problem is actually a *technical* one – we need to make this happen in code. As per our conversations on automatic differentiation, we know how to do this: we code up our program using a framework for automatic differentiation that has defined primitives and gradient rules. `pyhf` Heinrich et al. (2021) is the software package that brings this to life: the whole HistFactory prescription, all coded using a choice of autodiff backends, e.g. JAX, TensorFlow, and PyTorch. There’s honestly not too much else to say here; any further discussion would involve extremely niche and technical topics within the `pyhf` codebase, and all the error messages I saw over the years I worked on trying to hack things together. I’ll spare you that discussion (feel free to ask about it, or [browse the pyhf issues on the topic](#)), and we’ll move on to something a little more thesis-suited (though, what is a PhD if not niche and technical...).

7.2.5 Differentiable test statistics (profile likelihood ratio)

Recall from Section 3.3 that when we’re constructing test statistics, we’re using the building block of the *profile likelihood ratio*, which we state once again as

$$\lambda(x, \mu) = \frac{p\left(x|\mu, \hat{\theta}(\mu)\right)}{p\left(x|\hat{\mu}, \hat{\theta}\right)}.$$

The variables $\hat{\theta}(\mu)$ and $\hat{\mu}, \hat{\theta}$ are the result of two separate maximum likelihood fits. Are these differentiable? Well, yes – we can leverage the utility of automatic differentiation to trace each iteration of the optimization loop at runtime, and then do the corresponding gradient calculation by composing VJPs and the like. However, that could get really expensive as the number of iterations gets into the thousands, which isn’t too uncommon in practice. Do we have a way to get around this?

Thanks to the groundwork we set up in Section 5.3, we worked out that we can take the gradient of **fixed points** (e.g. solutions to minimization algorithms) through a simple analytic formula in terms of the update step f , the solution of the optimization problem θ_0 (or $\hat{\theta}$), and some particular value of $\varphi = \varphi_0$ that we used to define the objective:

$$\frac{\partial \theta_0}{\partial \varphi_0} = \left[I - \frac{\partial f}{\partial \theta_0} \right]^{-1} \frac{\partial f}{\partial \varphi_0}. \quad (7.7)$$

What does φ mean here? It corresponds to the *same* φ that we’re talking about in this section (the notation was not a coincidence)! Specifically, these would be the *analysis configuration*

parameters (e.g. a combination of neural network parameters, observable binning, cutflow, etc.), which all *implicitly* determine the form of the likelihood. The language of “implicit” refers to the fact that we build the likelihood using the counts of the histograms for each physics process, with those counts in turn being influenced by φ , but we do not explicitly denote the likelihood as $p(x|\mu, \theta, \varphi)$, for instance.

In practice, we can implement this through moving the goalposts for what we call a primitive: for optimization loops like this, we can define that as a primitive of sorts, and then give it the known gradient as defined by Equation 7.7. This is the kind of approach taken by `jaxopt` (Blondel et al. 2021), which is a library that’s used a few times in this thesis.

7.2.6 Differentiable hypothesis tests

What’s left to get us over the line to differentiating the result of a hypothesis test? Well, thanks to the formulae outlined in Section 3.3, to extract the expected (read: median) p -value from the observed value of the test statistic $t(x_0)$, we only need to do one last simple algebraic calculation:

- For the **discovery p -value** with test statistic q_0 : $p_0 = 1 - \Phi(\sqrt{q_0})$.
- For the p -value associated with setting an **upper limit** using test statistic q_μ : $p_\mu = 1 - \Phi(\sqrt{q_\mu})$.
- For the **CL_s method**, we can just compose the p -values from the previous step using different values of μ in q_μ as the point null: $\text{CL}_s = p_{\mu=1}/(1 - p_{\mu=0})$.

All of these formulae are differentiable without any extra work, so we’re done!

7.2.7 Bonus: Uncertainties on likelihood parameters

Recall from Section 2.2.1 that the *Fisher information matrix* $\mathcal{I}(\theta)$ gives us access to the covariance matrix for maximum likelihood estimates, provided we’re in the asymptotic limit, through the Cramér–Rao bound:

$$\Sigma_{\hat{\theta}}^2 \geq [\mathcal{I}(\theta)]^{-1} .$$

Since $\mathcal{I}(\theta)$ is defined in terms of second-order derivatives of the log-likelihood – something that we’ve already made differentiable from a code perspective – we can then calculate the Fisher information using automatic differentiation. Moreover, since function transformations like the gradient operator are composable in automatic differentiation frameworks, this will itself be differentiable! This gives us access to many other inference-aware quantities that we can use as both diagnostics and as loss functions, including diagonal elements of the covariance matrix, which correspond to the individual uncertainties on each likelihood parameter. This

approach was first explored by INFERNO (Castro and Dorigo 2019), from whom we take much inspiration from in this section.

Now, the fisher information involves a matrix filled with second derivatives of the likelihood, and so requires data and parameters to be evaluated as a number. One thing we can do in the HistFactory setting is use Asimov data, which would mean we'll be able to know the best-fit parameter values already, and we can attempt to achieve the Cramér–Rao bound in Equation 2.7 by evaluating at $\mu = \mu'$, $x = x_A(\mu')$. As to the choice of μ' , I'm not sure that it matters too much, as we're always going to be at the best fit parameter value for μ (the likelihood shape itself isn't affected by this, for instance), but I haven't studied this in detail.

7.3 Putting it all together!

Now that we've enabled the differentiability of all the components layed out in Equation 7.3, we can see what happens when we use the p -value as our loss function, i.e. use gradients in Equation 7.4 to update the parameters φ .

As a first example, we can look at the simple analysis from Section 7.1.1 as a candidate to test this out on! We were looking for the value of ϕ that corresponds to the best expected sensitivity to the signal model. Crucially, we needed to make sure that we accounted for the systematic uncertainty on the background σ_b , which heavily influenced the resulting optimization. Let's see if we can do that!

The results of training this setup to optimize ϕ with respect to the discovery p -value can be seen in Figure 7.16. Immediately, we can see that we've managed to find a point that minimizes the objective we care about, being able to incorporate uncertainty all the while! One thing I really like about this plot is the way it appeals to intuition – the expected counts that result from this procedure appear to be exactly at some medium compromise between signal to background ratio and uncertainty on the background. The acquired Swede within me would even go as far as to call it “lagom” – not too little, not too much; just the right amount³.

7.3.1 A quick aside on INFERNO vs neos

My advocacy hereafter is to refrain from using `neos` or INFERNO methodology naming, since these methods differ only on small implementation details, the main one being the *choice of loss function*.

One interesting thing to note: we're calculating the expected discovery p -value using the asymptotic formulae outlined in Section 3.3. Minimising this p -value corresponds to pushing the observed value of the q_0 test statistic as far to the right as possible (i.e. maximizing its

³If you're less of a holistic person and would prefer something more quantitative, you can see a real-life carving of the “lagom” amount in Lund, just outside one of the main university buildings.

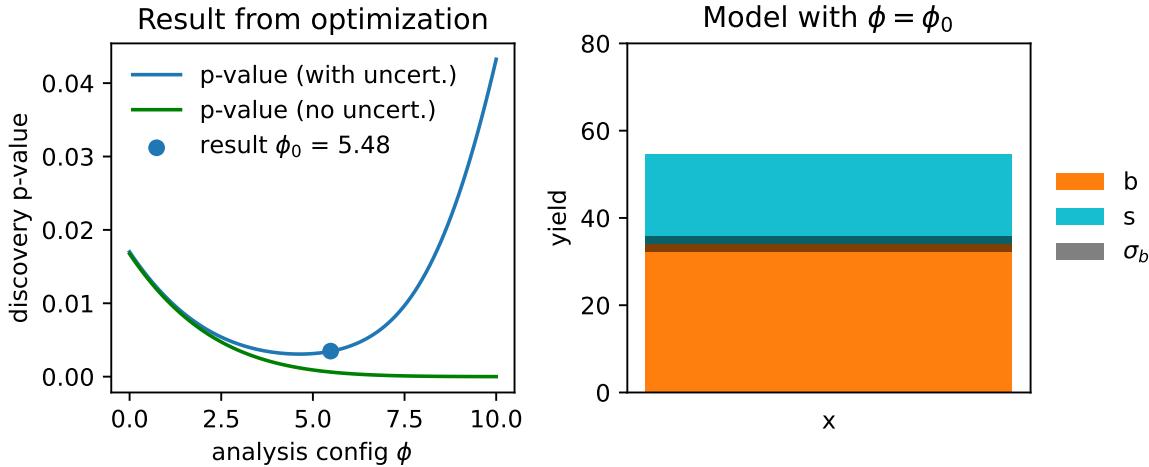


Figure 7.16: Left: The resulting point from optimizing ϕ with gradient descent. Right: The histogram model at the solution of the optimization.

value), which will trap smaller and smaller proportions of the distribution $p(q_0|\mu_0)$ (smaller p -values). Recall that Equation 3.6 states that we know an interesting fact about this test statistic: it's approximately equal to $((\mu_0 - \hat{\mu}(x))/\sigma_{\hat{\mu}})^2$. Since we're using Asimov data with $\mu' = \hat{\mu} = 1$, and probing a null of $\mu_0 = 0$, the test statistic is actually an (inverse) estimate of the variance of $\hat{\mu}$, which is being minimized during optimization! This has a lot of similarities with INFERNO, since both methods are effectively minimizing the same quantity, but estimated a different way; INFERNO uses the Fisher information estimate, and `neos` uses asymptotic formulae.

If we were to apply this same logic to calculating a p -value (or a CL_s value) for upper limit setting, then we'd instead be using q_μ , and would typically examine Asimov data with $\mu' = \hat{\mu} = 0$ (no signal) while looking at a null of $\mu_0 = 1$. We would then still end up with the same relation of inverse proportionality to $\sigma_{\hat{\mu}}^2$. Of course, the test statistics q_0 and q_μ differ conceptually in their definition, so there are likely going to be differences in practice if we used one or the other for optimization (but we would definitely expect a reduced uncertainty on $\hat{\mu}$ in either case). We'll see these differences in practice later on.

Equipped with these systematic-aware (or more aptly, *inference-aware*) loss functions, we can now apply them to something a little more complicated.

7.4 neos: End-to-End Optimized Summary Statistics for High-Energy Physics

This section summarizes the work I've done in the paper (Simpson and Heinrich 2021). New follow-up studies will be shown in later sections.

The problem of reducing a whole set of physics quantities into a single number, or **summary statistic**, is not a new one in HEP. The reason for this is two-fold: inference in high-dimensional settings is computationally difficult, and the probability model defined by the underlying physics is intractable to explicitly compute. This leads to practice referenced a few times already, where we construct models via HistFactory, which are almost always based a single quantity, e.g. something like the invariant mass of the final state you're interested in, or the output of a machine learning model. In the latter case, we're typically concerned with optimizing for discriminating signal and background processes. However, we know from the previous sections that we can do much better by optimizing with respect to a p -value, especially when we have significant systematic uncertainties to worry about.

To be more concrete: we'll look at optimizing a neural network-based summary statistic for a simple HEP-like situation, including the construction of the uncertainty through interpolating between “up” and “down” variations of the background. We'll refer to this workflow as **neos**⁴, with the full proposed pipeline shown in Figure 7.17.

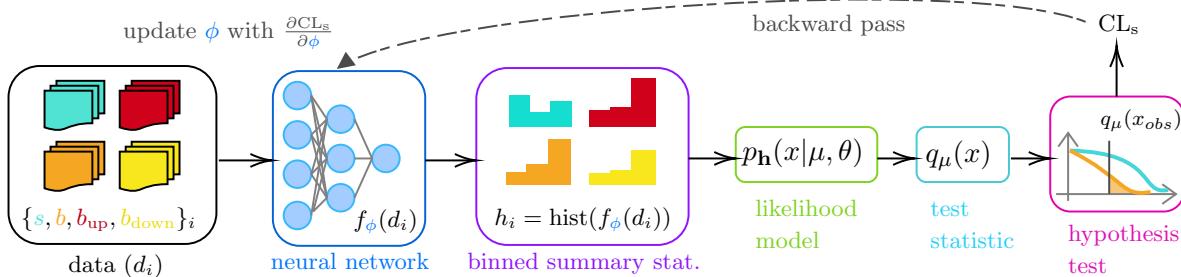


Figure 7.17: Outline of the workflow proposed for **neos**.

7.4.1 Example: Gaussian blobs

Pretending our detector only outputs two physics variables x and y , we'll generate some toy data from different 2-D normal distributions (“Gaussian blobs”) for both signal and background, making sure they overlap a bit as to not be trivially separable. We'll then also sample from Gaussian blobs on either side of the background, and treat these as “up” and “down” variations

⁴Originally an acronym for neural end-to-end optimized statistics, but acronyms are annoying, so I don't really make that explicit anymore. Hopefully the rest of this section will also convince you that we don't need to get too caught up with naming anyway.

in the way described in Section 3.2.2. We can see the result of sampling 10k points for each blob in Figure 7.18.

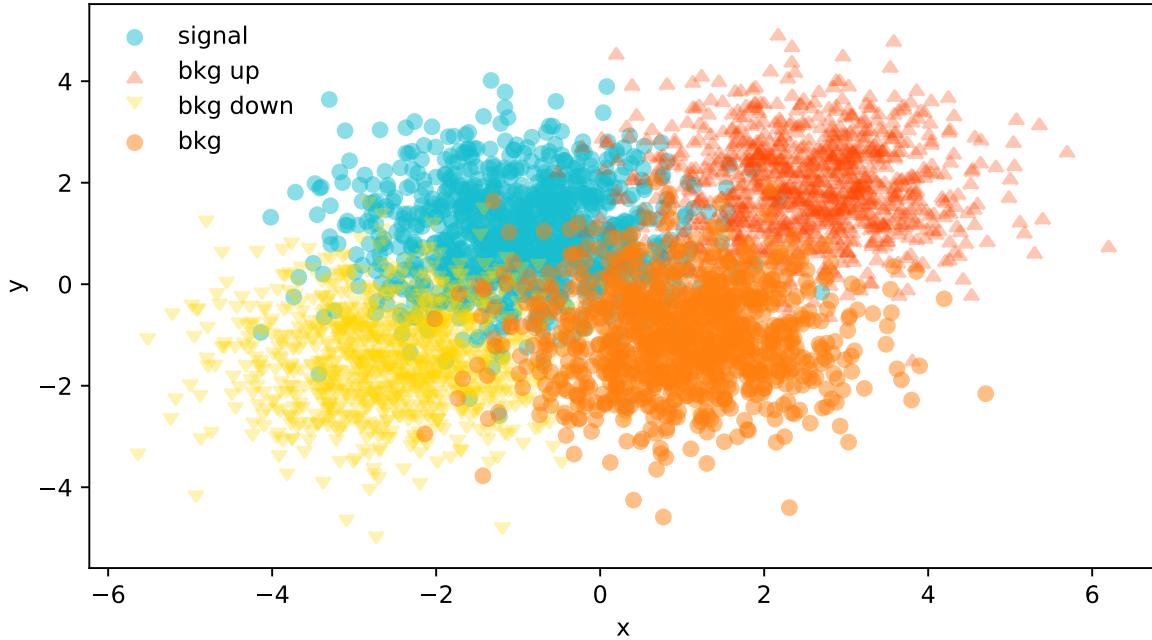


Figure 7.18: Plot of 10k samples from toy distributions representing imagined signal, background

From here, things follow the diagram in Figure 7.17:

- We'll pass the samples of x, y values for each blob through a neural network, which turns each tuple of (x, y) into a single number $f_\varphi(x, y)$, where f_φ is our current network with parameters φ .
- We'll then have four sets of values of f_φ for each blob (signal, nominal background, and the up and down variations of the background), which we then turn into four histograms. During optimization, this histogram will be a bKDE as per Section 7.2.3 to make the final loss (CL_s) differentiable, but we'll replace it with a regular histogram for calculating our evaluation metrics.
- Using these histograms, we'll build a HistFactory statistical model in exactly the same fashion as Equation 7.2 – with one parameter for the signal strength μ , and one nuisance parameter γ that's constructed by interpolating the shape variation between the histograms of the nominal, up, and down variations of the background.
- We then build the appropriate test statistic based on this likelihood, and perform our hypothesis test – not on the observed data (we don't have any), but on the Asimov dataset for that hypothesis (i.e. for a null of $\mu = 1$, we're going to use the dataset that would result in $\hat{\mu} = 1$ when fitting the likelihood, which would just be the nominal counts $s + b$).

- The final step is producing the end result of that test (e.g. CL_s), then taking the gradient of that whole chain, which we'd use to update the parameters of the neural network φ .

We'll feed data in using mini-batches, and hold out a group of points for each blob as a test set, which we use to calculate metrics and select the best model (normally we should never use the test set to choose a model, but the distributions are simple enough that there will be almost no macroscopic difference between train, validation, and test sets). The histogram yields are all divided by the number of data points per-batch, and then re-scaled to be on the order of tens of events, with different factors being applied to signal and background to put us in a more realistic regime (e.g. of low signal and high background).

In the graphs about to be shown, we'll benchmark `neos` against optimization against some other loss functions:

- **Binary cross-entropy** (BCE): This will try to discriminate signal versus nominal background samples, and will not be informed about the up/down samples during training.
- **BCE with data augmentation**: As above, but we indiscriminately label all of the background samples with one label instead of using just the nominal (this should be a very powerful baseline).
- **INFERNO**: As in Section 7.2.7, we'll take our loss to be the diagonal element of the inverse Fisher information that corresponds to the signal strength μ .

Results (as shown in the `neos` paper)

The full set of hyperparameters for this study are:

- 10000 data points, split evenly between all four blobs,
- 3-layer neural network of size (1024, 1024, 1),
- Training with Adam optimiser, learning rate 1e-3,
- Adam optimiser also used in maximum likelihood fits with learning rate 1e-3,
- $m_s = (-1, 1)$, $m_b = (2.5, 2)$, $m_{b\text{up}} = (-2.5, -1.5)$, $m_{b\text{down}} = (1, -1)$,
- Multiplicative histogram scale factors: signal scale=2, background scale=10, global scale=10,
- ReLU activations, with sigmoid activation on the final layer,
- 15 epochs, with a batch size of 2000.

Results from the training process using these hyperparameters are shown in Figure 7.19, where each curve is the average of that metric across 7 different training runs, all with unique random initializations of the neural network parameters. The figure has three plots, which we'll cover from left to right. Note: these quantities are all computed on the same *test set* (unseen data), and use no approximations to hard operations in their calculation (which basically means the histogram is a normal one for `neos` and INFERNO).

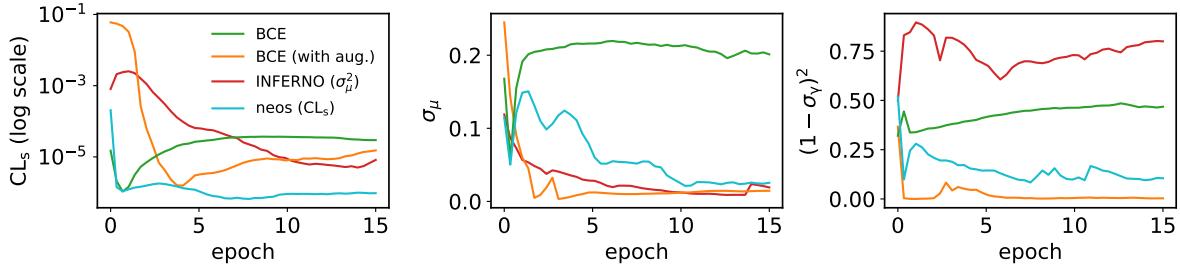


Figure 7.19: Results from training neural networks using the four loss functions highlighted in the legend. Left: the expected CL_s . Middle: The uncertainty on the signal strength μ . Right: The deviation from the nominal width of the nuisance parameter γ that controls the background uncertainty.

The leftmost plot contains the expected CL_s for all four methods. We can see that the absolute lowest value of this is only attained by `neos`, which makes sense – we’re using this as the loss function itself. Both BCE methods reach a fairly low value quite quickly, which can be attributed to the fact that it’s not that difficult to isolate most of the signal in this example. Interestingly, INFERNO demonstrated far less stability with its CL_s value, with the different training runs having quite large variance in this quantity, causing their average to perform quite poorly. This says more about the interplay between the uncertainty on the signal strength and the CL_s than it does about what we consider “good performance” – I’ll come back to this in the discussion.

The middle plot is the uncertainty on the fitted value of the signal strength $\sigma_{\hat{\mu}}$, as calculated through the Fisher information. Something I think is cool here is that `neos` learns to minimize this over time without any explicity prompting to do so (we’ll discuss more on this later). It’s no surprise that INFERNO does very well here, as again, it’s trained precisely to do so. BCE with augmentation also does very well, which is likely because we’ve ensured that anything that is non-signal looking, including possible variations on the background, is pushed to one side of the histogram, and the signal, which can be well isolated, is pushed to the other. Regular BCE, however, does okay initially, but will quickly overfit to the nominal signal/background discrimination if left to train for longer, which won’t care if there’s high background uncertainty in the signal bins.

The final plot on the right shows the squared deviation from the nominal uncertainty on the background nuisance parameter γ , which we acquire through the appropriate diagonal term in the inverse Fisher information. In the likelihood modelling stage, this uncertainty also has an associated constraint term of $\text{Normal}(0|\gamma, 1)$, where the “units” of γ are chosen such that γ_{nom} sits at 0, and $\gamma_{\text{up}}/\gamma_{\text{down}}$ lie at ± 1 respectively. If the standard deviation of the fitted value $\hat{\gamma}$ is different to 1, we then have a contradiction between the fitted model and the implied uncertainty from the constraint term. This is known as over/under-constraining the parameter (depending if the uncertainty is smaller/bigger than 1), and can be associated with model misspecification (although there are cases where it is perfectly reasonable to constrain

the nuisance parameter depending on the nature of the measurement). Plotting this term (or $(1 - \sigma_{\hat{\gamma}})^2$ to just show the deviations) is then a useful diagnostic to see the learned behaviour of the observable with respect to the nuisance parameter. Training with CL_s doesn't appear to introduce any pathologies in this regard, and in fact appears to further reduce dissonance between the constraint term and the Fisher information with more training. This is also the case for BCE with augmentation, but vanilla BCE and INFERNO don't appear to exhibit this behaviour, and instead show some differences with the modelled standard deviation. The fact that BCE has no awareness of the background variations makes this less surprising, but I understand this less well for INFERNO at the time of writing (or even if it's a problem at all).

7.4.2 Practical issues

Regardless of any results, one immediate concern that you may have thought of while I talked about `neos` was the scaling aspect. We can't escape that one forward pass and one update step is computationally equivalent to two runs of the whole analysis inference chain (remembering that gradients from autodiff are of the order of the forward pass to `calculae`). In practice, this seemed to be around $\sim 3\text{-}4x$ an increase in performance time for an update to complete compared to BCE, but I'd expect this to increase more when applied to real analyses due to the complexity of the model, which has to be built each time for every set of new parameters⁵, and also will have a much larger number of parameters, which will impact the speed of calculating the profile likelihood.

Another issue is that these inference-aware metrics require enough data to produce a reasonable reflection of the actual analysis model. With a very small batch size, this is impossible; for medium-size batches, it may be that some kind of proportional scaling needs to occur so the yields maintain the same relative sizes, as was done in practice during the Gaussian blobs example (not using these scale factors actually makes training unstable).

7.5 What's *really* the best loss function?

The work done in making CL_s differentiable opened up a variety of new inference-aware losses as a by-product, including but not limited to:

- CL_s (and its associated p -values)
- p -value for discovery (p_0)
- Quantities derived from the Fisher information matrix of the full HistFactory likelihood, such as:
 - uncertainty on the signal strength σ_μ

⁵I did some work on trying to cache these models and update them in-place – if you're interested, see [this pyhf issue](#)

- deviations from the nominal nuisance parameter uncertainty, e.g. $(1 - \sigma_{\gamma})^2$
- the generalized variance, defined as the inverse determinant of the Fisher information
- Deviations from the nominal values of the nuisance parameters from control measurements (“pulls”)
- ... and *any algebraic combination of the above!*

Indeed, since all of these quantities can be calculated in a differentiable way, we can create a hybrid loss function using any of these components, such as $a_1 \text{CL}_s + a_2 \sigma_{\mu}^2 + a_3 \log p_0 + \dots$ etc. We can even view this through the lens of regularization, where we have one clear loss target, then introduce other components weighted with small linear coefficients to steer away from potentially undesirable pathologies.

Amongst those metrics already mentioned, one further example of a quantity that could serve this purpose is the empirical notion of the “**Gaussianity**” of a likelihood, which my colleague/supervisor Lukas Heinrich coined as the mean-squared difference across a grid of points between the learned HistFactory likelihood and a Normal distribution defined using the covariance implied by the (inverse) Fisher information matrix (remember the Cramér–Rao bound from Section 2.2.1). This would essentially control the validity of the assumptions made when using the Fisher information to calculate uncertainties, as well as potentially reducing the chances of arriving at poorly-behaved likelihood shapes that happen to satisfy a low value of any particular metric.

But despite all of this, I find myself a little bit torn as to the real answer to the question posed in the section title: which loss function is *really* the best for physics analysis? This inquiry brings us one layer deeper philosophically, as it touches on a more delicate question: how do we actually gauge how good a physics result is? We’d maybe say something that aligns with our physics goals, e.g. the discovery significance, but the way we assess analyses is a little more nuanced than this in reality. One can see this by thinking about reviewing an analysis paper – we’re not just interested in the significance alone, but also things like the pull plots, the validity of the modelling assumptions, whether things are correlated in the right place, and probably many other things that I’m not thinking of. Moreover, these nuances would be even *more* important if the significance was high!

As a very preliminary exploration of this question, we’ll look at an example problem where the “best” solution is clear. We can then attempt to construct a loss function that is convex in the region of the optimum.

7.5.1 A loss landscape interlude for a two-bin model

The problem we’ll look at is as follows: similar to the Gaussian blob problem, we’ll define a two-bin HistFactory model with a signal strength μ and a three-point uncertainty on the background γ . This model will be constructed from fixed nominal signal and background yields of $s = [5, 11]$ and $b = [50, 50]$, with two free parameters u and d that control the up and down

variations: $b_{\text{up}} = [50 + u, 50 - u]$, $b_{\text{up}} = [50 - d, 50 + d]$. The intuition for this is that any change in u or d will asymmetrically affect each bin by the same amount, so any optimization can't focus on the gains from just one of the two bins. When both u and d are equal to 0, we'll have $b = b_{\text{up}} = b_{\text{down}}$, i.e. no systematic uncertainty on the background. We know that this would be the ideal solution, but what do our metrics have to say about it?

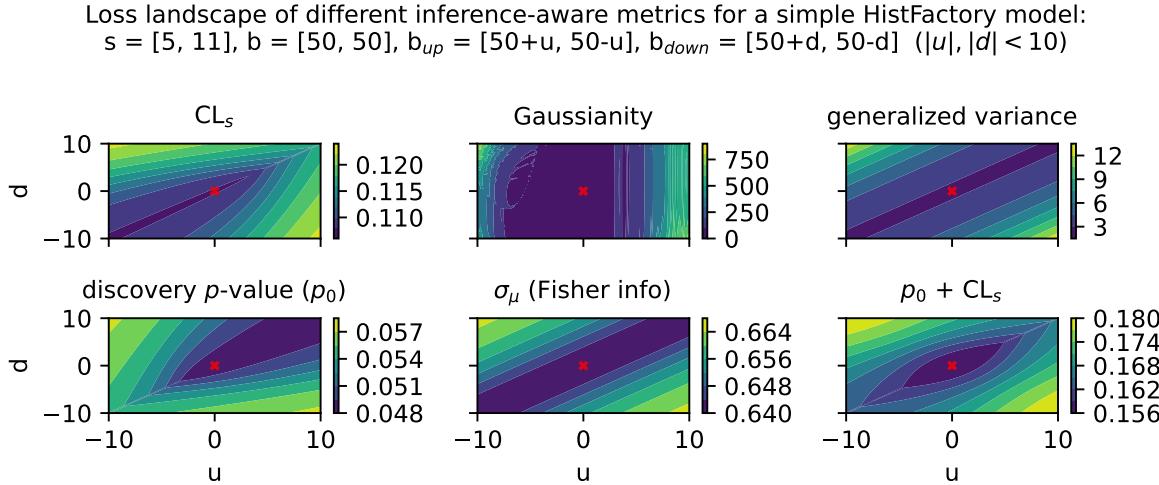


Figure 7.20: A scan over the loss landscape for a two-parameter physics model, with each parameter having an asymmetric contribution to “up” and “down” variations of the background. The point $[0,0]$ corresponds to no uncertainty on the nominal background prediction, and is highlighted with a red cross to indicate the target solution.

Figure 7.20 shows a scan over the loss landscape for many of the metrics we’re interested in, including the various p -values, signal strength uncertainty, and a few bonus metrics that haven’t been explored (Gaussianity and generalized variance).

The first thing that I’ll guide your eyes to is the striking asymmetry in the CL_s and p_0 landscapes. For each individual metric, the asymmetry arises from the uneven signal distribution across the bins. The pattern we see is as follows: both metrics enjoy when u and d are approximately the same (which can be said for pretty much all the metrics). However, we then see the asymmetry: CL_s prefers u and d to be more negative (corresponding to up/down background variations below nominal in the first bin, and higher than nominal in the second), and p_0 prefers u and d to be more positive (up/down variations below nominal in the second bin, and higher in the first). As to why this is, my first thoughts are that the role of $\mu = 0$ and $\mu = 1$ switches between the two metrics: for discovery, we’re testing a hypothesis of $\mu = 0$ on Asimov data for $\mu = 1$, and for CL_s , we’re testing $\mu = 1$ using Asimov data for $\mu = 0$. Then, in some way, the bin with the lower signal contribution (first bin) is more important for low CL_s , and the higher (second bin) is more important for a low discovery p -value. This explanation certainly appeals

to intuition in some ways – particularly that the discovery p -value wants the background variations as low as possible in the high-signal bin – but perhaps warrants examination through a more quantitative lens in future work.

One surprising artefact of the asymmetry between CL_s and p_0 is that a simple addition between them produces something fairly bowl-like around the point $u = d = 0$, which we consider desirable from the perspective of an optimization procedure being able to achieve that minimum in practice. We can see this plot in the bottom-right of Figure 7.20, though it's possible that one may want to match the scales of both quantities in practice by doing some weighted combination, which would make it so that one objective is not largely preferred over the other (e.g. here, something like $\text{CL}_s + 2p_0$ would approximately match their absolute values). Of course, we should keep in mind that this apparently useful behaviour may vanish with more model complexity, and also requires fitting the same model twice for each forward pass if we're calculating two profile likelihoods.

As for the other metrics, they generally become lower when u and d become more equal, corresponding to $b_{\text{up}} \approx b_{\text{down}}$. Interestingly though, there isn't much preference to the absolute values of the up and down variations, as long as they're equal. This is a little counterintuitive, as we'd expect everything to benefit more in the case of $b = b_{\text{up}} = b_{\text{down}}$ (i.e. when $u, d = 0$), or at least have some kind of different result depending on the size of the variations compared to the nominal background prediction. However, one interesting pathology I discovered when looking more closely at these metrics is that they all have the *exact same values* along the line $u = d$. This line also happens to be where the minimum values of the metrics lie, which is even true for CL_s and p_0 . It's particularly hard to see this effect in Figure 7.20, so I've extrapolated just that line for all the metrics and plotted it in 1-D, shown in Figure 7.21. This is where Gaussianity can perhaps find utility: it's the only quantity that varies asymmetrically along this line, and has a series of minima close to $u = d = 0$. All other metrics retain exactly the same values for all models along the line, even those with values of $b_{\text{up}} = b_{\text{down}}$ that differ from the nominal by 10 in each bin. We'll see little bit of this behaviour to prefer $b_{\text{up}} = b_{\text{down}}$ over $b_{\text{up}} = b_{\text{down}} = b$ in the next section, where we revisit the `neos` example of Gaussian blobs through the lens of examining the relationship between the metrics.

7.6 Gaussian blobs, again

Inspired by the studies in the previous section, I thought it would be useful to try the study from the `neos` paper a second time, but with some additional loss functions that we haven't touched on yet (e.g. the discovery significance). Moreover, it may be illustrative to track the values of all the possible loss functions for each training strategy. In this way, we'll be able to capture some idea of the relationships between quantities of interest – at least within the scope of the example itself.

We'll look at the following choices for the training objective:

Values of metrics along the line $u = d$ (+ Gaussian noise for line visibility)

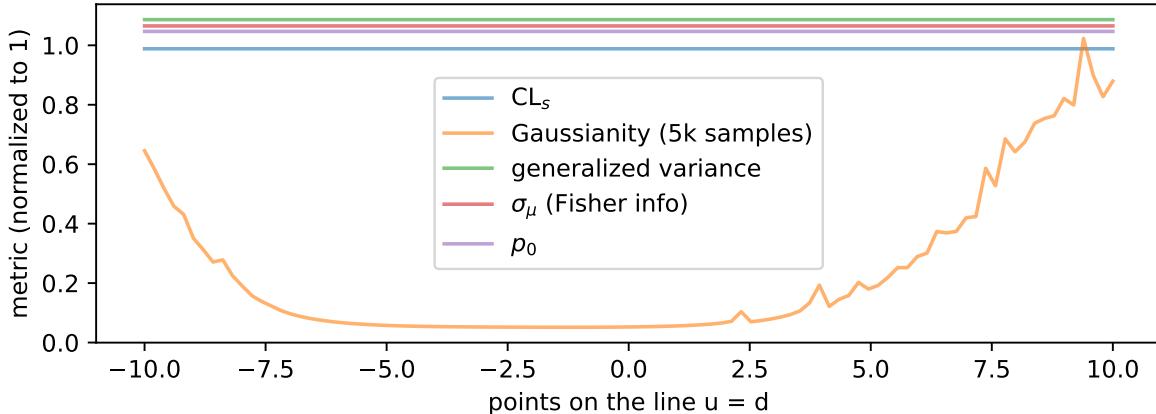


Figure 7.21: A projection of the line $u = d$ for all metrics, which are normalized by their maximum value. A small constant noise value is added to each metric in order to see all the lines at once.

- BCE with data augmentation (serving again as a strong baseline)
- CL_s
- p_0
- σ_μ
- $CL_s + p_0$ (inspired by the previous section)

The pipeline is exactly the same as in Section 7.4, but with slightly different hyperparameters. The only ones that differ are:

- 5-layer neural network of size $(128, 128, 128, 128, 1)^6$
- More epochs (~ 100) with the same batch size of 2000 to view the learning process over a longer period of time (it looks like some curves in Figure 7.19 would keep reducing with more training)
- Average over nine random seeds (previously seven – just a time constraint on both accounts)
- Bandwidth of 0.09 for the bKDE, found through trial and error by making it as small as possible while still producing stable training runs

As an additional layer of complexity, we'll look at how the different training strategies perform when using a lower and higher number of bins for the neural network observable, to see if that

⁶Initially, this was chosen to be less wide to maybe slow down the learning process a touch, though the extra layers mitigate that to some degree. It turned out that this made the training much more stable for some reason (less variability in the metrics), so I kept it.

influences the efficacy of the methods. The bandwidth should then in theory be shrunk in proportion to match the smaller bin widths, though

7.6.1 5-bin observable

Metrics

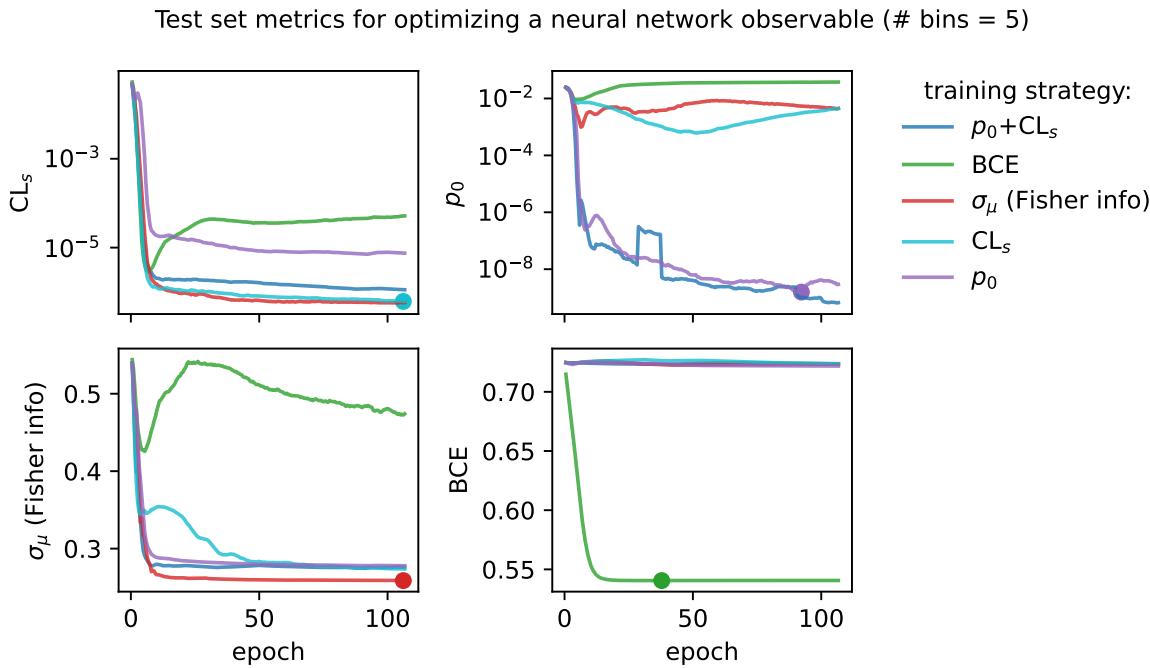


Figure 7.22: Plots of the different metrics calculated on the test set for different training strategies using a 5-bin neural network observable. The results are averaged across 9 random seeds for the weight initializations. The scatter points on some of the curves represent the model that we would select in practice if using that training strategy (provided we decide to use the loss as the selection metric).

We'll start by looking at the overall metrics when optimizing a 5-bin observable. These are shown in Figure 7.22, where the circular points show the epoch where we would stop training and select that set of models across all the random seeds (being loose with the distinction between validation and test sets in this toy problem setting). To recap the differences to Figure 7.19: we're using a slightly different neural network (deeper & narrower), training for longer, and tracking all the different metrics for each training strategy.

By looking at the various metrics, we can see that training to minimize binary cross-entropy quickly converges to its best performance, since it's not too difficult to separate the nominal

signal and background samples from each other in data space (teal vs orange points). It's worth pointing out that the small minima that appear early on in the three inference-aware metrics aren't actually attained by the "optimal" solution that we decide on from looking at BCE alone. Even if we don't train using those metrics, it then may still be worth tracking them to choose the best network.

When comparing BCE to other training strategies, note the difference in discovery p -value – apparently we miss out on a p -value that's better by *six orders of magnitude* (a difference of $\approx 4.75\sigma$ for those that prefer significance) if we choose BCE over something like p_0 as an objective! It's also interesting to note that there's a very weak correlation between the models that are more inference-aware and their respective binary cross-entropies.

Another identifiable difference I'll highlight is that training to minimize σ_μ is *much* better than it was in the `neos` paper! It also follows a curve that resembles that gained from optimizing CL_s for most of the metrics, which is much more in-line with expectations: remember that minimizing CL_s will also minimize some version of σ_μ too! So why were they so different in the `neos` paper? Well, the reason I seemed to stumble upon is that the wider and more shallow network of size (1024, 1024, 1) produces results with much higher variance for some reason when trained to optimize σ_μ . This is reflected in a statistic I didn't show in the initial `neos` studies – the networks trained with different random seeds for the network parameters had very high variance! Why this occurred for σ_μ in particular is unclear to me, but the results with the narrower, deeper network used here are far more stable, which will be seen again when we dive into some of the resulting models.

As to why the Fisher information estimate of σ_μ minimizes CL_s much more than p_0 , there are a number of potential causes. Here, we evaluate the Fisher information using Asimov data with $\mu' = \gamma' = 1$, i.e. the nominal signal + background hypothesis; earlier I said it shouldn't matter too much what this choice is, but it could play a factor that CL_s also uses this Asimov data configuration. It could also stem from the fact that $q_0 \neq q_\mu$, but that's pure speculation at this point – this should be studied further in future. The one definite takeaway is that all these metrics care about minimizing σ_μ in some fashion, even if their mutual relationships are more complicated.

Commenting on other features: the new player in the game is the discovery p -value p_0 , which performs pretty well in the three inference aware metrics. It's curious to note that choosing CL_s or p_0 as a training strategy limits the performance in the other to a degree, though this is alleviated when training using their combination $CL_s + p_0$ (as would be expected). There is a saying though – when one uses a metric as a training objective, it ceases to function well as a measure of performance, so we should take this all with a grain of salt and some lemon zest. In some ways this saying is only partially true here, as these metrics are calculated using a regular histogram instead of a bKDE, so they differ in a mild conceptual way. But despite that, all of CL_s , p_0 , and adding them together seem to perform identically with the value of σ_μ they end up with.

There's a couple of good performances that are worth highlighting – optimizing with respect to σ_μ seems to match or beat using CL_s as the training goal within its own metric for one! It could be that it's an easier metric to minimize in practice, and so it reaches its optimal value much faster. Though, neither CL_s nor σ_μ seem to be super great at optimizing for p_0 (but they handily beat binary cross-entropy). Using $CL_s + p_0$ also ends up with a slightly better p_0 by a small amount than using p_0 as the objective, while not compromising on any of the other metrics.

As a supplement to the metrics we just examined, it's interesting to see the types of observable that the network learns for each metric. For this, I've plotted the resulting histograms for each training strategy that were learned by the best-performing models over each random seed. These histograms are further augmented by plots of the value of the neural network observable across data space, where the contours used are exactly the same as the bin intervals; you can do a one-to-one comparison by looking at the points enclosed in one contour, and find the bin that corresponds to that interval, where you'll see those points accumulated (after scale factors are applied). Many plots are ahead, and we could talk about them for a long time, but they're mainly there to try to give you the maximally verbose version of this study – some brief summative comments are provided that point out some of the features I notice to aid your mental dissection.

Consistent shapes of learned histograms are found in most metrics, with p_0 showing the most variability. You'll notice that sometimes the order of the bins appears to flip – that's purely based on the nature of the random seed, and which side shows higher significance first during training. In many of the inference-aware metrics, we see a lot of bins that try to balance the up and down variations of the background, which were shown to be the best-case performance for our two-bin model in Section 7.5.1. Moreover, this is apparently a more important condition for CL_s and σ_μ than it is for p_0 ; the former tend to favor an even spread of equal up and down variations across all bins, while the latter seems to prefer isolated signal bins with no events from background or variations thereof.

In the neural network contours, e.g. in Figure 7.29, we can see again the effect of p_0 aggressively trying to isolate the signal within the contours, whetheras CL_s and σ_μ prefer contours with balanced contributions from the up and down variations. The general pattern though in most cases is that the contours appear to curve around the signal for our inference aware metrics, whether as binary cross entropy just tries to draw a good dividing line between the orange (background) and teal (signal) blobs.

7.6.2 20-bin observable

Now we can see what happens when we provide a lot more bins to play with!

Example models learned when optimizing BCE (# bins = 5)

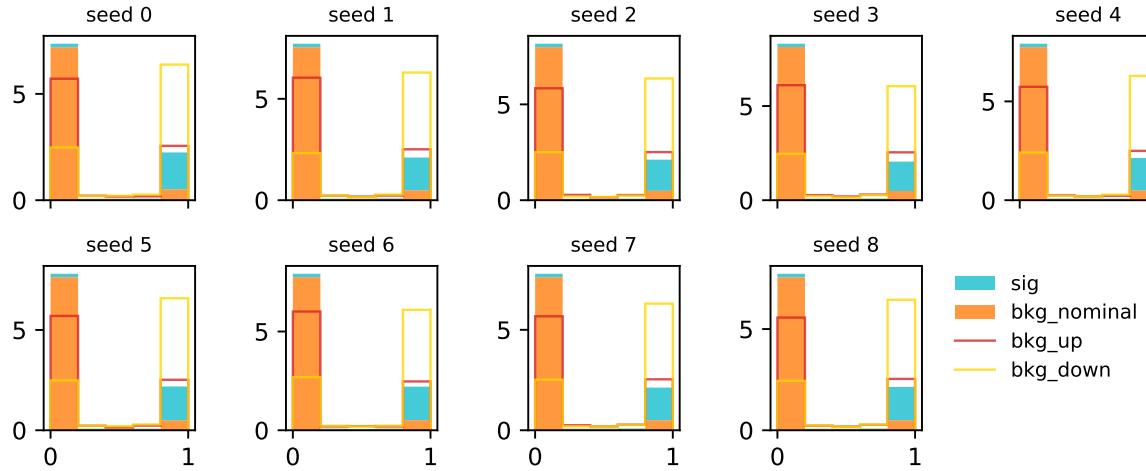


Figure 7.23: Histograms from optimizing with respect to binary cross-entropy between signal and nominal background.

Example models learned when optimizing p_0 (# bins = 5)

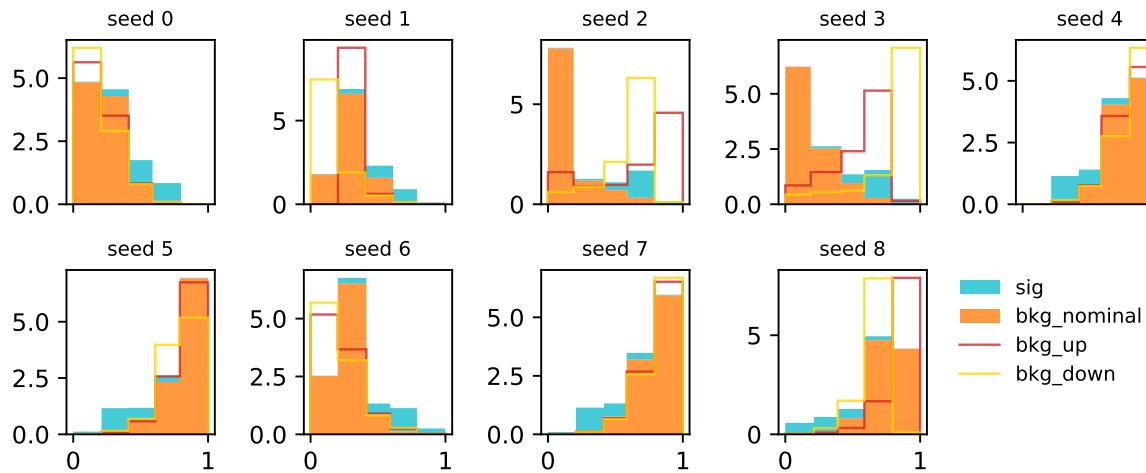


Figure 7.24: Histograms from optimizing with respect to the discovery p -value p_0 .

Example models learned when optimizing CL_s (# bins = 5)

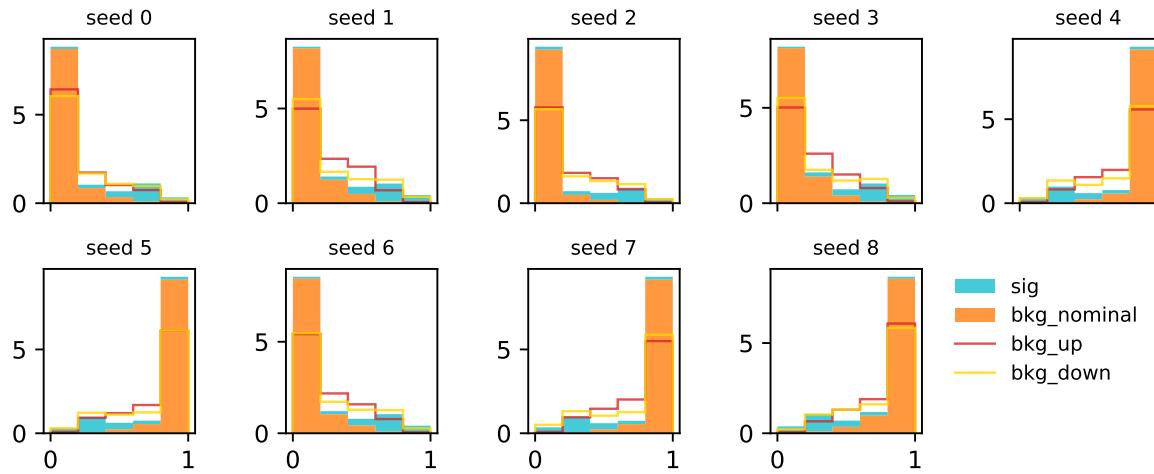


Figure 7.25: Histograms from optimizing with respect to the CL_s .

Example models learned when optimizing $p_0 + \text{CL}_s$ (# bins = 5)

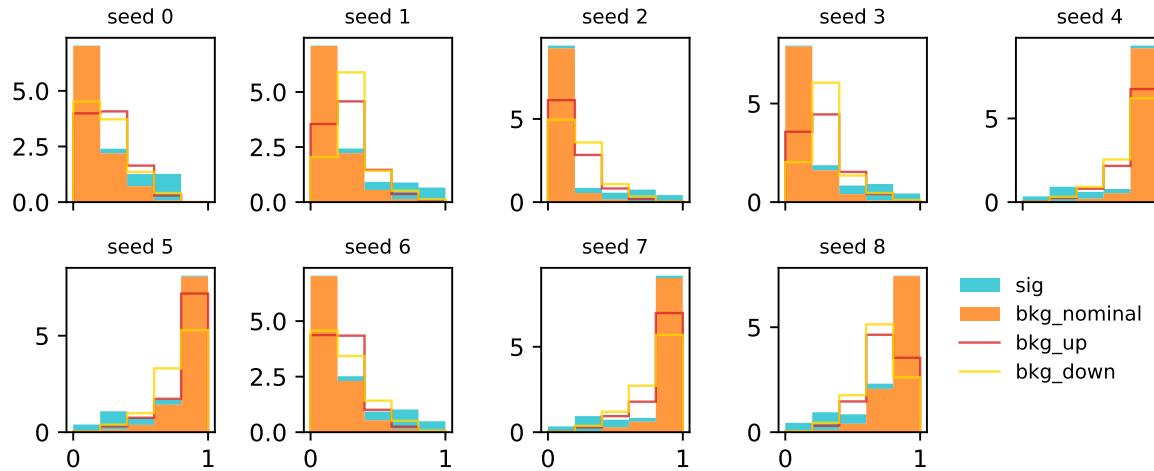


Figure 7.26: Histograms from optimizing with respect to a combination of discovery p -value and CL_s .

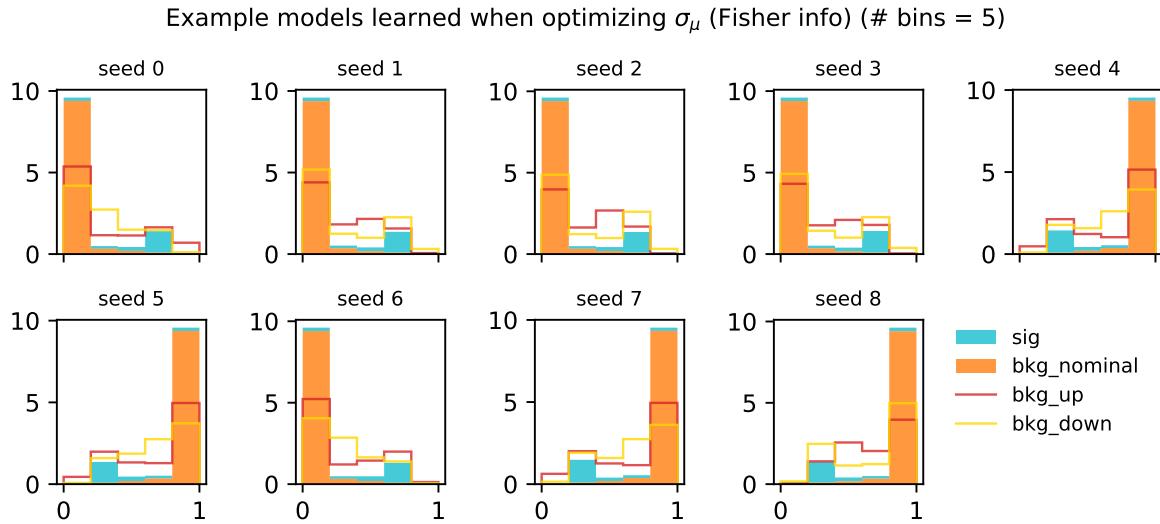


Figure 7.27: Histograms from optimizing with respect to the Fisher information estimate of $\sigma_{\hat{\mu}}$.

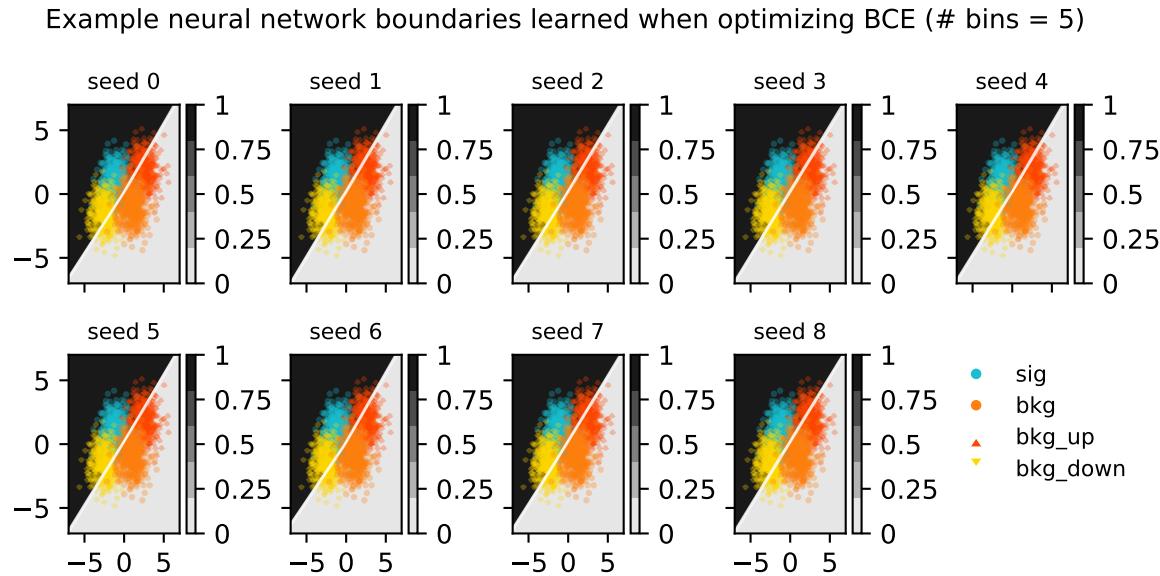


Figure 7.28: Contours of the neural network output from optimizing with respect to binary cross-entropy between signal and nominal background. The test set points are overlaid.

Example neural network boundaries learned when optimizing p_0 (# bins = 5)

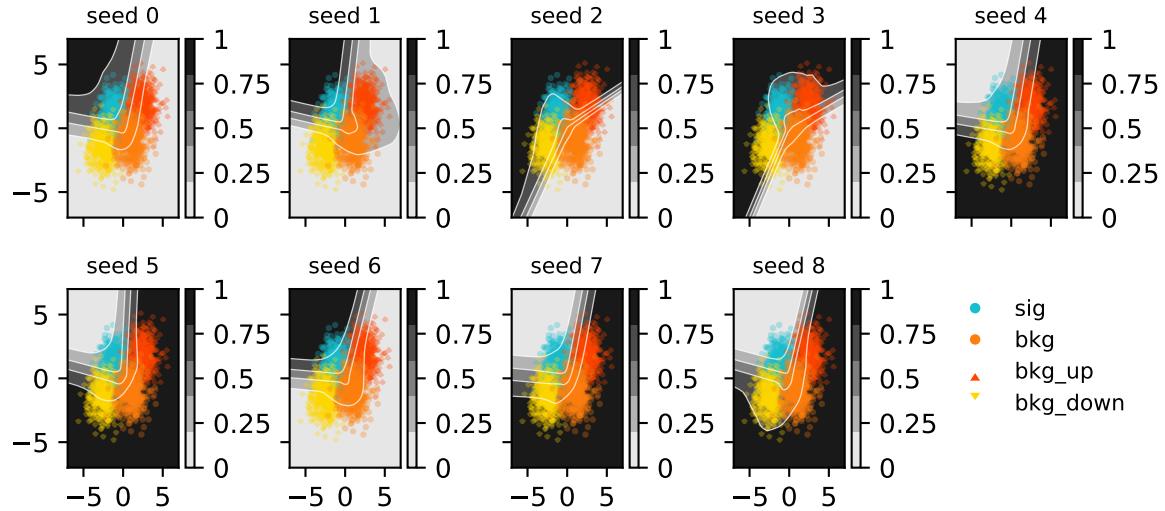


Figure 7.29: Contours of the neural network output from optimizing with respect to the discovery p -value p_0 . The test set points are overlayed.

Example neural network boundaries learned when optimizing CL_s (# bins = 5)

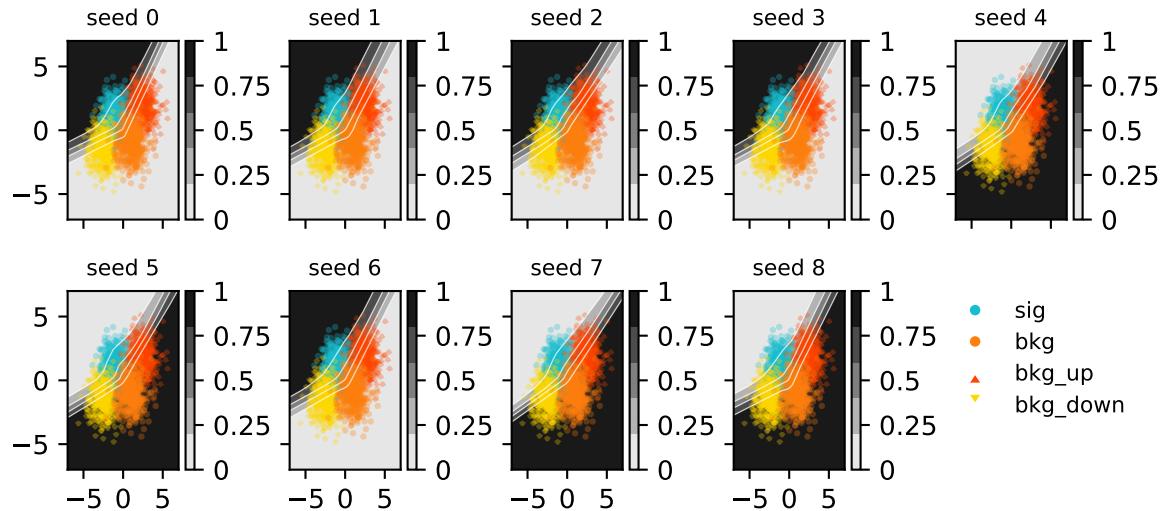


Figure 7.30: Contours of the neural network output from optimizing with respect to the CL_s . The test set points are overlayed.

Example neural network boundaries learned when optimizing $p_0 + \text{CL}_s$ (# bins = 5)

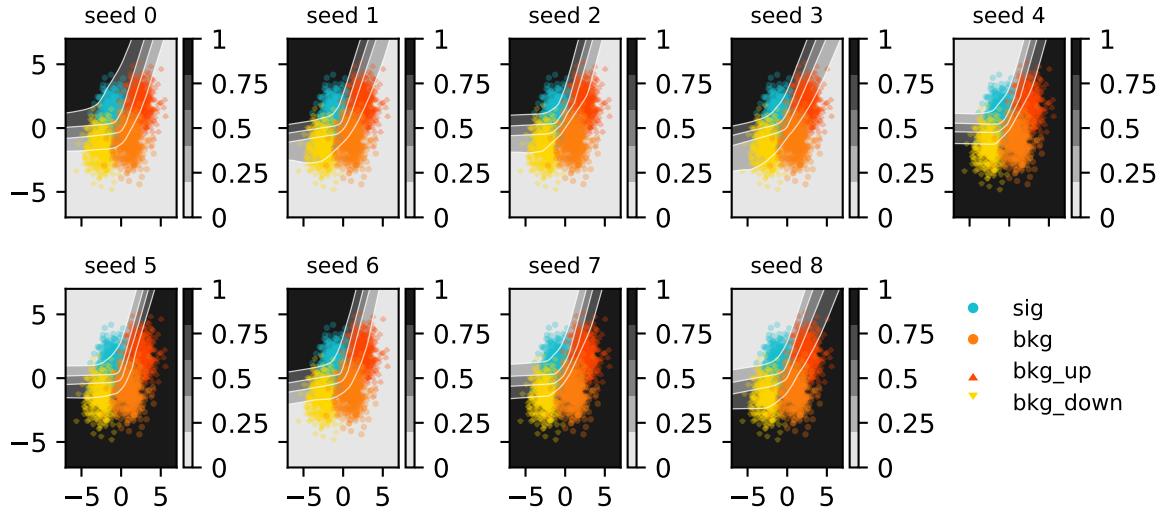


Figure 7.31: Contours of the neural network output from optimizing with respect to a combination of discovery p -value and CL_s . The test set points are overlayed.

Example neural network boundaries learned when optimizing σ_μ (Fisher info) (# bins = 5)

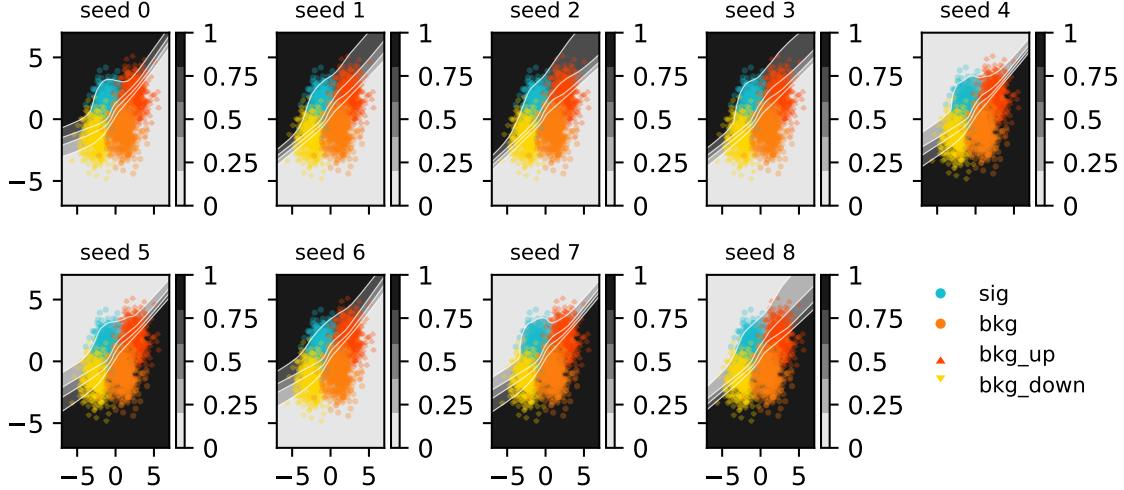


Figure 7.32: Contours of the neural network output from optimizing with respect to the Fisher information estimate of $\sigma_{\hat{\mu}}$. The test set points are overlayed.

Test set metrics for optimizing a neural network observable (# bins = 20)

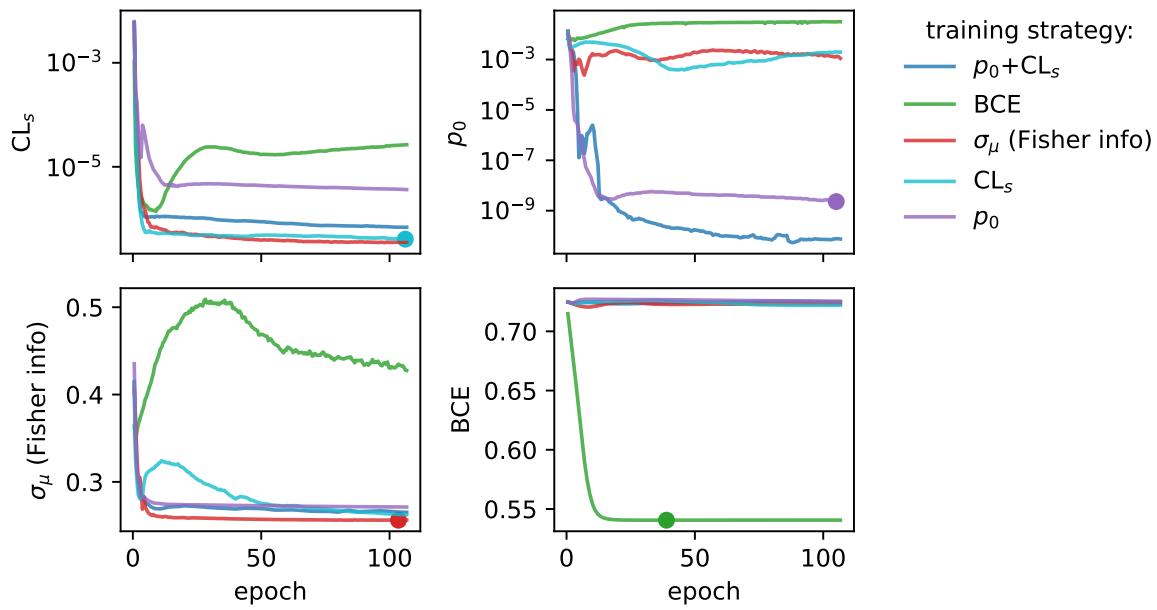


Figure 7.33: Plots of the different metrics calculated on the test set for different training strategies using a 20-bin neural network observable. The results are averaged across 9 random seeds for the weight initializations. The scatter points on some of the curves represent the model that we would select in practice if using that training strategy (provided we decide to use the loss as the selection metric).

Metrics

The story doesn't change too much with more bins, with all the training strategies maintaining their mutual relationships as discussed earlier. The only marked difference is that $p_0 + CL_s$ outperforms p_0 alone much more clearly here, which is pretty interesting to think about.

I'll also show the histograms and neural network contours in data space – there are some pretty funky ones for the high-bin case. You'll see that the types of histogram model learned by the neural network fluctuate much more with this additional granularity provided by the new bins, especially for the hypothesis test-based metrics (seed 2 and 3 are particularly strange for p_0).

For the contours themselves, there are many things to see here, but I'll just point out one of my favourites: for seed 3 in Figure 7.36 and Figure 7.35, we see the network struggling to untie the systematic variations from the signal bins. However, for the same seed in Figure 7.37, where we're training on a combination of those metrics, the network seems to manage! No idea why this behaviour is there, and indeed it is just one seed. But I thought that was pretty cool.

Example models learned when optimizing BCE (# bins = 20)

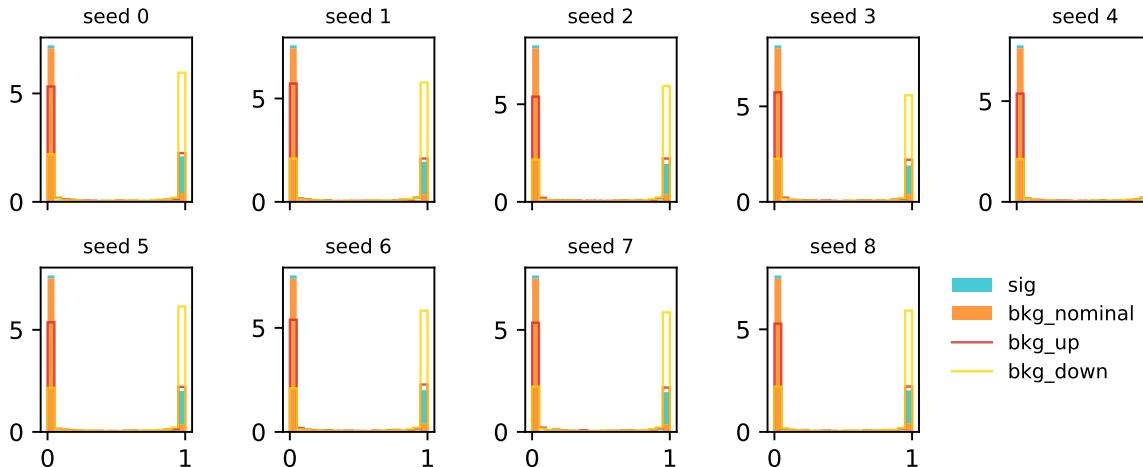


Figure 7.34: Histograms from optimizing with respect to binary cross-entropy between signal and nominal background.

7.6.3 Optimizing binning and neural network simultaneously

One thing I also thought to try is, for a fixed number of bins, exploring what happens when the bin edges are made to be *part of the optimization itself*. Our free parameters are then $\varphi = \{\varphi_{nn}, \text{bin edges}\}$. To prevent the bin edges from being non-ascending, a `jax.numpy.where` statement was used to replace values that were larger than their neighboring edge with something just below it instead. As opposed to bin edges, we could have equivalently let the bin widths

Example models learned when optimizing p_0 (# bins = 20)

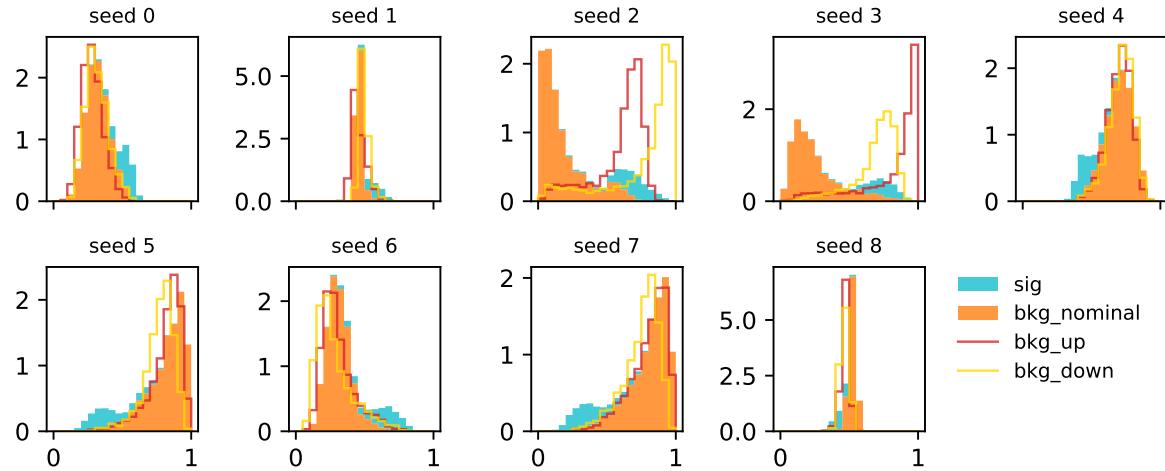


Figure 7.35: Histograms from optimizing with respect to the discovery p -value p_0 .

Example models learned when optimizing CL_s (# bins = 20)

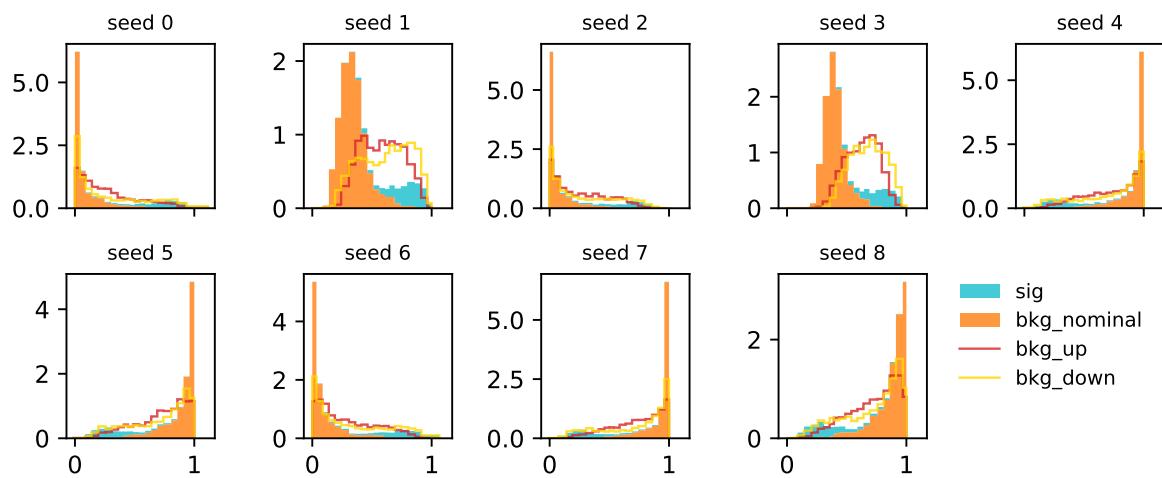


Figure 7.36: Histograms from optimizing with respect to the CL_s .

Example models learned when optimizing $p_0 + \text{CL}_s$ (# bins = 20)

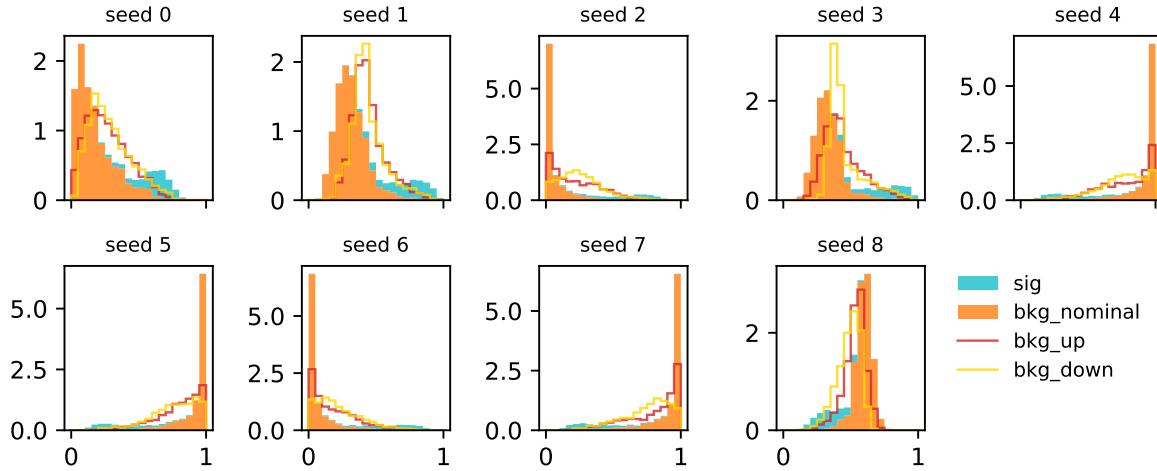


Figure 7.37: Histograms from optimizing with respect to a combination of discovery p -value and CL_s .

Example models learned when optimizing σ_{μ} (Fisher info) (# bins = 20)

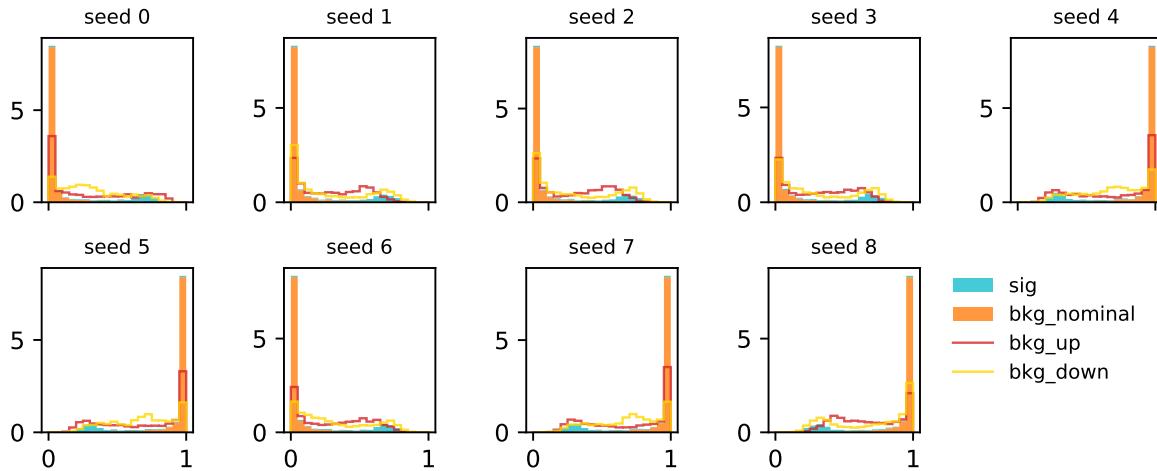


Figure 7.38: Histograms from optimizing with respect to the Fisher information estimate of $\sigma_{\hat{\mu}}$.

Example neural network boundaries learned when optimizing BCE (# bins = 20)

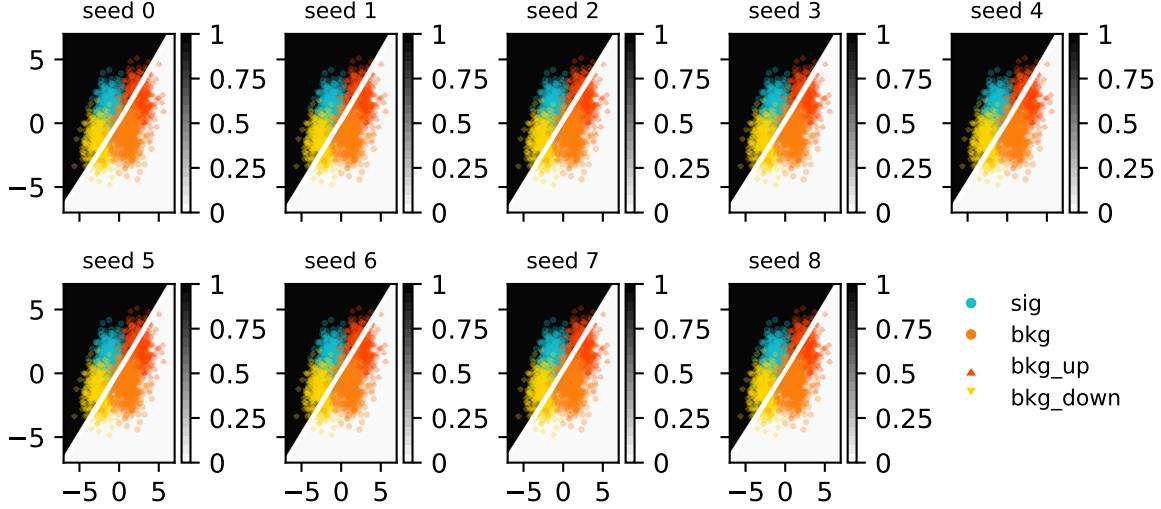


Figure 7.39: Contours of the neural network output from optimizing with respect to binary cross-entropy between signal and nominal background. The test set points are overlaid.

Example neural network boundaries learned when optimizing p_0 (# bins = 20)

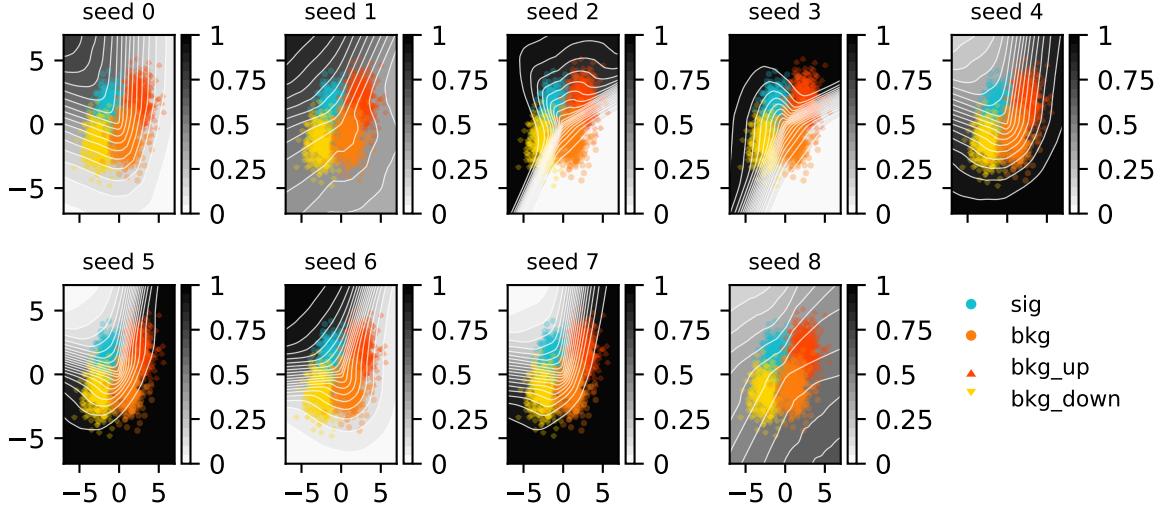


Figure 7.40: Contours of the neural network output from optimizing with respect to the discovery p -value p_0 . The test set points are overlaid.

Example neural network boundaries learned when optimizing CL_s (# bins = 20)

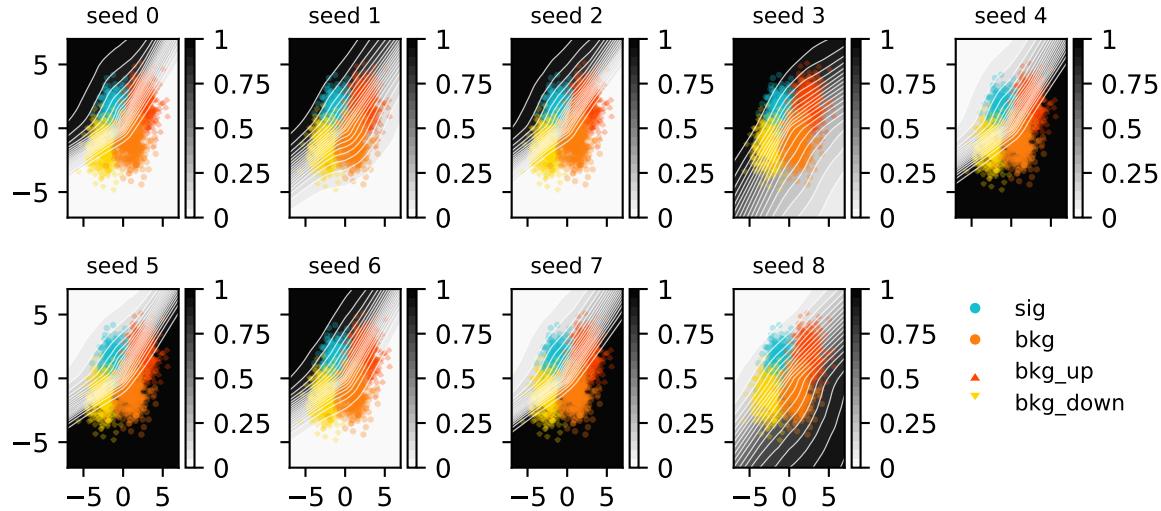


Figure 7.41: Contours of the neural network output from optimizing with respect to the CL_s .
The test set points are overlayed.

Example neural network boundaries learned when optimizing $p_0 + \text{CL}_s$ (# bins = 20)

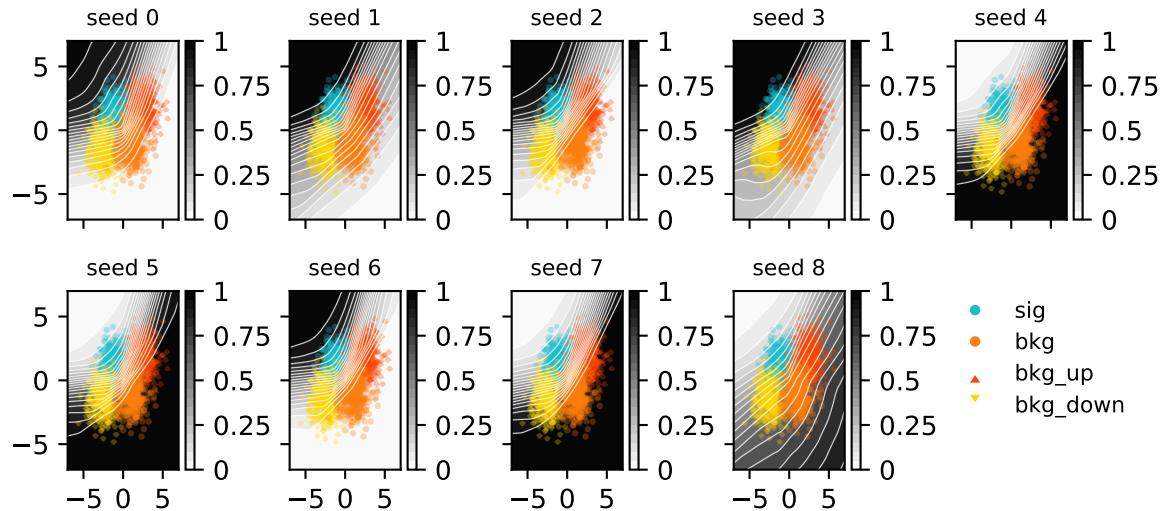


Figure 7.42: Contours of the neural network output from optimizing with respect to a combination of discovery p -value and CL_s . The test set points are overlayed.

Example neural network boundaries learned when optimizing σ_μ (Fisher info) (# bins = 20)

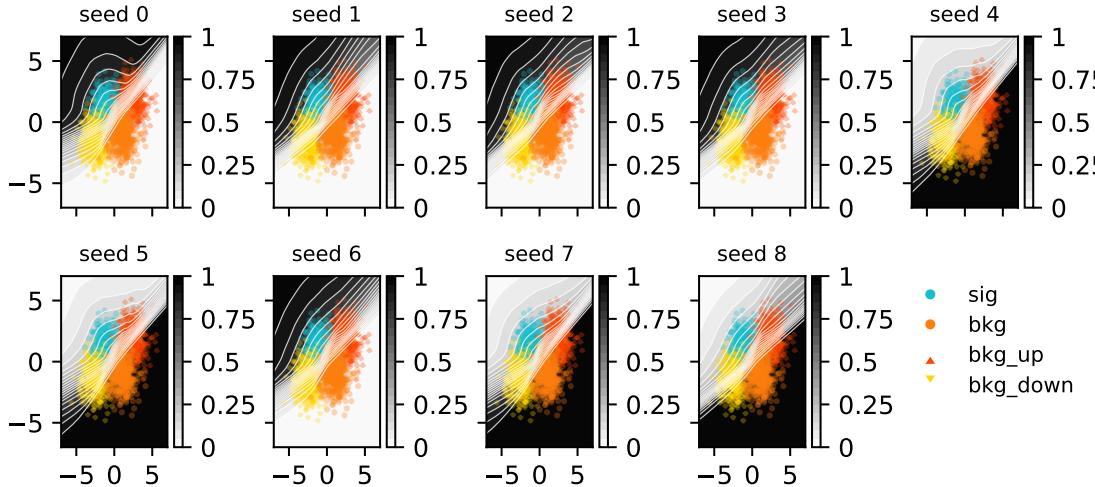


Figure 7.43: Contours of the neural network output from optimizing with respect to the Fisher information estimate of $\sigma_{\hat{\mu}}$. The test set points are overlayed.

vary instead, and decide the last width as $1 - \sum_{i=0}^{\text{number of bins}-1} \text{bin widths}_i$. In practice, this was found to be less stable when tried (often the sum of widths would exceed 1, and the last width becomes negative in that case). The endpoints [0, 1] were taken as fixed to ensure there isn't optimization that accounts for the bKDE spilling out outside that range. In hindsight, though, I think things would be fine without this restriction, especially since the best network is selected based on the the version of the loss with no approximations (i.e. a pipeline that uses a regular histogram with the optimized binning).

Results from this experiment are fairly similar to the fixed-bin case, and are shown in Appendix A. The most notable finding is that $\sigma_{\hat{\mu}}$ seemed to be the metric that made use of adapting the binning the most, but didn't necessarily translate this to a big performance gain.

7.7 What's next?

The first question that arises when reading this work for most – which mirrors accurately the same question I get when giving talks about this – is *how does it scale to optimize with a p-value?* Great question; I wish I knew. I've not personally managed to apply this to a real use-case where this method could thrive (e.g. a physics analysis where systematic uncertainties serve as a bottleneck for performance). But if we were to do so, scaling will come with some challenges: the first being that the accuracy of the model construction per iteration is dependent on the batch size being large enough to faithfully represent the analysis. In practice, this

was overcome by applying scale factors to the batches that normalized their event counts to something expected by the whole sample (in our toy case, we made the arbitrary choice of a 1/5 ratio between signal and background, with a normalization to around ~ 10 events or so). Moreover, the unavoidable truth already mentioned in Section 7.4.2 is that the cost of the forward pass + backward pass = $\sim \mathcal{O}(2 \times \text{analysis cost})$, which may scale in complicated ways depending on the complexity of the model at hand. One would probably need to prune any workspace to only include systematic uncertainties that have been studied to impact the analysis result significantly.

A whole world of things could be targets for being made differentiable. As a simple extension to what's already been shown here, one could imagine making upper limits differentiable in the same way as the profile likelihood; there's no conceptual restriction, but since there's an optimization procedure to determine the upper limit (find the value of the parameter that gives a certain p -value), we can reuse the idea of implicit gradients that exist for functions with fixed points. There's also a nice [set of operations that could benefit from being differentiable](#) curated by Kyle Cranmer, including things like sorting, statistical methods, and peer review (perhaps more relevant after AI take over the world – we can optimize their weights to help us get accepted at major conferences)⁷. It's possible that I've gotten around to implementing some of these in `relaxed` (Simpson 2022a) by the time you read this, which is a differentiable toolbox of sorts that implements all of the advances that you've seen in this chapter.

While we're on the topic, one particularly cool thing about `relaxed` is that it mimics the APIs of commonly used software tools in HEP. As an example, hypothesis tests are usually done with `pyhf` using the one-liner

```
pyhf.infer.hypotest(
    mu_0,  # null hypothesis for mu
    data,
    model,
    test_stat,  # = q_mu or q_0
)
```

And indeed, the same call works for `relaxed`, with the bonus being you can differentiate the result:

```
relaxed.infer.hypotest(
    mu_0,  # null hypothesis for mu
    data,
    model,
    test_stat,  # = q_mu or q_0
```

⁷Thinking about it though, AI having a workshop about the workings of AI would be more like biology/philosophy. Perhaps this whole thesis is then unethical through this lens, exploiting and manipulating machines for our own curiosity. The complementary idea of inverting this exploitation is a rather dystopian one.

```
    lr = 1e-3 # learning rate for fits (done with grad descent)
)
```

To see more of what this looks like in practice, I encourage you to check out the [repository](#) (e.g. the [tests](#)), a [set of examples that I wrote](#) (Simpson 2022b), and my [PyHEP 2022 video tutorial](#).

Beyond quantities that stem from statistical inference, differentiable simulation is another promising area that could allow simulator-in-the-loop optimization. An example could be tuning your simulator parameters to model data by gradient descent, or perhaps having a pipeline with a loss function that simulates physics on-the-fly based on learned parameters. Moreover, there has been a very interesting recent line of work that looks at making key physics processes differentiable, such as the calculation of matrix elements for scattering amplitudes (Heinrich and Kagan 2022) and parton showering (Nachman and Prestel 2022). This is certainly an area to keep an eye on over the coming years.

7.8 Credits

Many thanks go to Lukas Heinrich for the inspiration, debugging help, and original proposal, and also to Tomasso Dorigo/Pablo de Castro for their initial assistance and work on INFERNO (Castro and Dorigo 2019), which lay lots of the groundwork for this topic. Thanks also to the other pyhf authors Matthew Feickert and Giordon Stark, and to Alex Held for his great notebook on differentiable cuts and other advice.

8 Signal Model Interpolation using Normalizing Flows

One of the primary goals of data analysis in collider physics is to test the viability of proposed models for new physics, which attempt to address the shortcomings of the well-tested Standard Model. We'll call these models the **signal**. Since we don't have access to real data from these hypothesized phenomena, we use high-quality simulations of the underlying physics to generate samples that mimic data collected from major experiments, e.g. the Large Hadron Collider. This then lets us identify the most prominent signature that physics process leaves in the data, such as the shape of the invariant mass of some particular final state. We can compare that signature with data generated to mimic the same final state, but with only standard model processes (which we term **background**), and use this comparison as a mechanism to produce an analysis that *could* discover the signal if it were present. This can then be applied to real data.

How many models are there to test? In general, there's no upper limit – arXiv grows thicker every day with more theory model submissions. But what about within a certain class of model with *similar free parameters*? This scope-narrowing makes our lives much easier, as we're only now limited by the parameters of the model, e.g. the mass of a new particle. One could then imagine testing each possible value for this new mass... until we realize that there's only so many times we can do this. Recall that simulating data is in general expensive, and we'd rather avoid it where we can. Moreover, if we have a multi-dimensional parameter space to explore, covering that in an efficient way will be prohibitively expensive to simulate. How do we get around this?

Well, if we're interested in some signature from the model in a particular set of variables, we could generate that data for a set of parameters, then find some way to interpolate between them. Specifically, this can be viewed as trying to estimate the probability density (or *shape*) of a variable of interest, where we want to *condition* on the physics parameters involved in the generation of that shape. This is the approach taken here.

It's worth noting that physics analyses typically don't interpolate on the level of the statistical model, and instead just interpolate the result of the search itself, e.g. in the space of p -values or on limits for the signal strength μ across a grid of e.g. different signal masses. This is often quoted without error (a different issue), and does not take into account the fact that we'd expect to be less sensitive to new physics in the regions that we don't have high-quality simulations for. However, if one can interpolate the signal model in some way *before* calculating the final

result, then incorporate a predictive uncertainty from that interpolation into the statistical treatment of the data, we should hopefully be able to have a more grounded representation of our sensitivity between simulated signal model points.

8.1 Problem statement

Say a simulated signal process outputs a set \mathbf{x} of per-event physics quantities (or **observables**), where each quantity is typically a real number (e.g. kinematics). We're interested in making a statistical model of this process, and so take interest in the distribution over \mathbf{x} , which we'll denote $p_s(\mathbf{x}|\theta)$, with θ representing the free parameters of the physical model (and s standing for signal). We can partition θ as $\theta = [\phi, \nu]$, where ϕ effectively parametrizes the hypothesis of the new physics model (e.g. through the mass of a new particle), and ν represents parameters that are needed to specify the physics conditions, but are not of interest (e.g. a jet energy scale). We focus on conditioning with respect to ϕ here, and leave treatment of ν as part of the statistical modelling process (see Section 3.2.2 for more on this).

We don't have a way to calculate this density due to our inability to access the implicit distribution defined by the simulator, but we do have access to the samples themselves (at some finite number of values of θ). This means we can empirically estimate the distribution in some way, provided we have the right tools to do so. If successful, we're free to directly use this empirical estimation of $p_s(\mathbf{x}|\theta)$, but in practice, we're often faced with an additional modelling constraint: many analyses in collider physics operate using *histograms* of observables, and construct a statistical model based on that. As such, it would be desirable if we could find a density estimator that:

- allows for the *conditioning* of side variables (here, this would be conditioning on ϕ)
- has a tractable likelihood (e.g. for direct use in “unbinned” analysis)
- can model discrete densities like a histogram
 - or, optionally, allow the generation of samples that can be histogrammed later
- (optionally) comes with a notion of uncertainty

This brings us to normalizing flows!

8.2 Normalizing flows (recap)

A much more extensive motivation for normalizing flows can be found in Section 6.2, but we'll recap the main points here.

Normalizing flows are a class of density estimation technique, which attempts to transform a designated *base* density into a *target density with the aid of neural networks. This admits the

ability to sample from a flow, since you can just transform the samples from the base density, which is usually of simple form (e.g. normal distribution). Moreover, flows have a tractable likelihood, which can be evaluated by transforming the samples using the learned transform, putting that into the base density, and multiplying by the relevant Jacobian, effectively bending the space into the desired shape to mimic the target density.

To train a flow, we simply fit samples from the base distribution to the training samples such that the negative log-likelihood of the flow model is minimized. This is done across batches of different training data, just as in standard machine learning optimization.

All of the properties of a flow satisfy most of the bullets above for our criteria, but we're still missing two parts: conditioning and uncertainty. These are addressed in the following sections.

8.2.1 Implementing conditional density estimation

A few different types of models allow for conditional density estimation, e.g. RealNVPs (Dinh, Sohl-Dickstein, and Bengio 2016), MADE (Germain et al. 2015), and masked autoregressive flows (MAFs) (Papamakarios, Pavlakou, and Murray 2017) – we focus on the latter as the choice for this task. Details on the precise implementation of a MAF can be found in Section 6.2.2.

8.2.2 Estimating predictive uncertainty

If we're using the likelihood (or a histogram of the samples) to make a prediction using the flow, we don't have a natural way to produce a corresponding uncertainty on that prediction. One way to get around this fact is to take inspiration from the notion of **model ensembles** (see a review in (Ganaie et al. 2021)), which combine multiple predictive models into one by averaging their predictions at a given point, then providing an uncertainty through the sample standard deviation across those predictions. The intuition behind this is that one would expect models to have the most mutual variance in the region where there is no training data, as that lies outside of the context that the models learned. There's no particular way in which one needs to form the different elements of an ensemble for it to have some reasonable utility, but one common strategy in the land of neural networks is to train a few models with different weight initializations, and use those as the models to make up the ensemble. This approach is what we do here: both with the likelihood functions, and with the histogram yields produced from samples of those flows.

8.3 Example 1: Following the mean

To test out the MAF as a conditional density estimator, it suffices to model some family of distributions parametrized by some context ϕ , just as we set out in the problem statement.

One thing I thought of when considering this is a 2-D normal distribution, where the mean represents the context. This should be a simple starting problem, and is a similar use case to that which I encountered in a physics context, where the signature left in the invariant mass spectrum clustered around the value of the rest mass of the particles that produced it. We'll add more complexity to this later.

We'll start by sampling a range of normal distributions with different means and unit covariance. The means here are the *context* – the thing we'll condition on during training and inference. Training data will then consist of pairs of samples from these distributions, and the mean of the distribution that generated the samples. We'll also split the different distributions up into context points that are used for training, and unseen points that are used for validation and testing (in practice, these should be two distinct tasks, but we'll combine them for these examples to portray the proof-of-concept in a best-case way). Points in the test set are not seen during training; we use them purely to assess performance (and select a good model) when interpolating to a context not seen before.

As a small note here, we also hold out a small number of examples (20% per point) from the training set to use as additional validation in conjunction with the unseen context points. These together are referred to as the “valid” set in the loss curve plots, and are used only for model selection purposes, including making sure we're not totally biasing our selection to the small number of unseen context points (we want to make sure performance on the whole grid is maintained). This is a hyperparameter that could be played with, or discarded altogether. More discussion on this can be found later on.

The distributions chosen are shown in Figure 8.1, where 49 different means have been evenly selected across a grid of points, indicated by crosses colored by the set they belong to. Note that the test set points are chosen such that they're all *inside* the grid – this is because we're seeking to interpolate our results within the region we have data as opposed to extrapolate outside of it.

10,000 points are then drawn from each distribution, and 3 MAFs are trained on the same training data, but with different weight initializations. The hyperparameters for training those MAFs are as follows:

- Batch size of 4000 points
- 10 layers of linear, autoregressive transforms
 - Each transform's neural network has one hidden layer of 6 neurons
- Adam optimizer with a learning rate of 1e-3
- 3000 iterations total (common reasonable plateau point for all examples)

During training, the inputs and context are each scaled to standard normal distributions through fitting a `StandardScaler` from Scikit-Learn (Pedregosa et al. 2011) to the train data. Any samples produced from the flow are then transformed back using this same scaler. Training

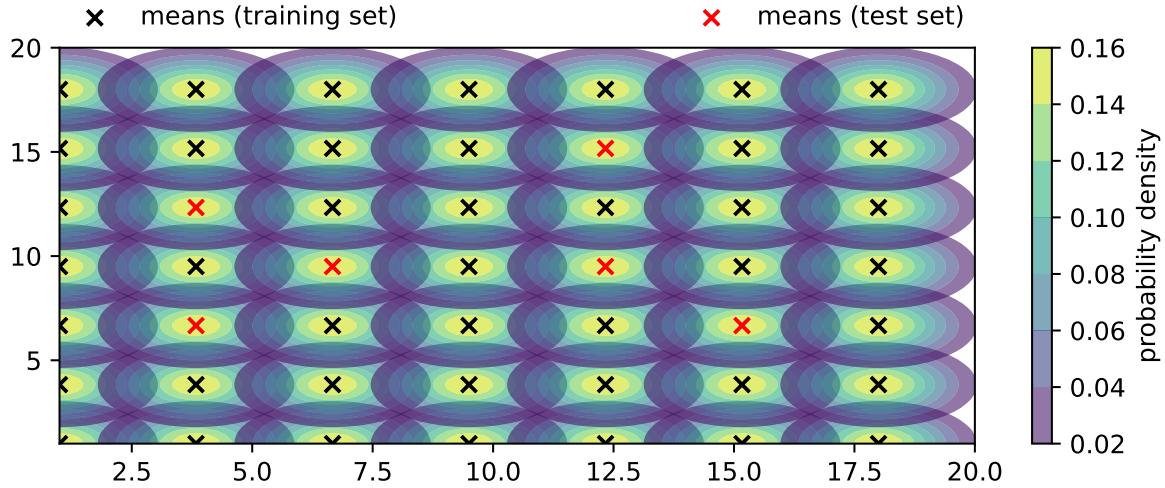


Figure 8.1: A grid of 49 different normal distributions, each with a mean corresponding to a cross on the image, and with unit covariance. The contour representing 0 is omitted for visualization purposes.

was done using the `nflows` software package (Durkan et al. 2020), which builds on PyTorch (Paszke et al. 2019).

It's worth noting that since we trained three MAFs, when I refer to the “flow” in later sections, I'm referring to the ensemble of all three models, where their predictions (either likelihoods or histograms) are averaged together, and their predictive uncertainty is the corresponding standard deviations.

We can examine the results of the training through different types of visualizations, as we'll see below:

8.3.1 Loss curves

See Figure 8.2 for a comparison of the negative log-likelihood loss for train and test sets. This is for just one of the three flows, and shows the similarity of the train and test losses due to the fact that the train and test data are so similar (there's not much domain shift needed, just learning the position of the mean).

8.3.2 Distribution similarity

It's illustrative to plot the likelihoods learned by the flow for each of the context points, including the ones for which we didn't see during training. We could, in theory, supply any

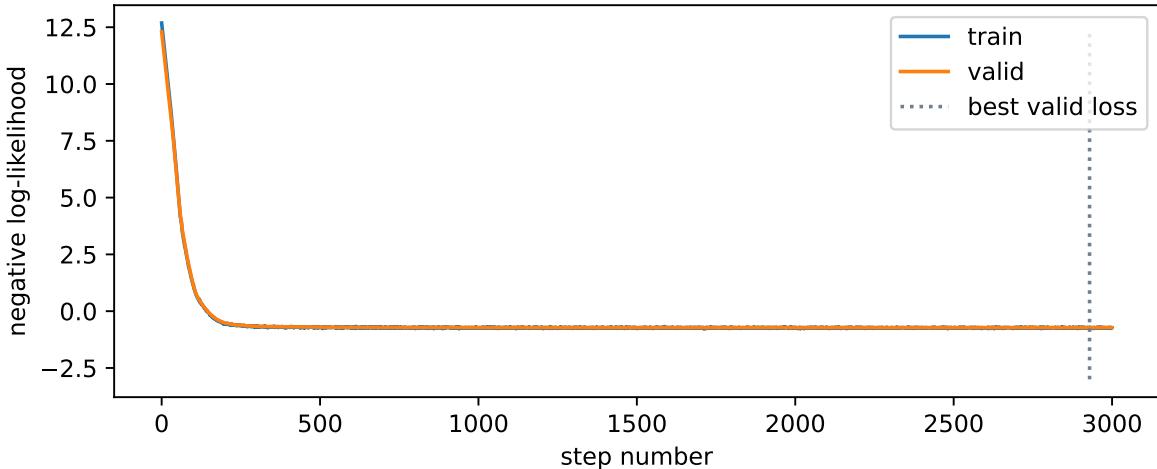


Figure 8.2: Example loss curves from a single flow trained on the “following the mean” scenario. The model weights are extracted from the best test loss.

value of the context for this evaluation, but it’s much more useful to do it in the region that we have test data so we can compare the result.

We can find this plot in Figure 8.3, where the plot from Figure 8.1 is shown as a comparison metric side-by-side. We can immediately see that the likelihood shapes are about what we’d expect, but we note the contours are coloured in log scale for the flow, which is done so to enhance visibility of the shape close to the mean, since the contours increase more rapidly in value around the center of the distribution. Additionally, the values of the normalization are much higher for the flow, which can be attributed to the fact that the training data is very concentrated around the mean, and so a distribution with all its density there will quickly give a good solution, as opposed to distributing that over a larger range in a more diffuse way. This could likely just be due to the training data being capped at 10k points.

This is a nice visual check, but it’s probably more useful to quantify this similarity in some way.

8.3.3 Histogram similarity

Since we’re interested in possibly using the result as a histogram, we can directly compare histograms of samples from the flow with histograms of the original data. Plots of the raw data versus flow differences can be found in Figure 8.4 for training points, and Figure 8.5 for test points. The plots are made using a histogram of the whole dataset for each context point (10k data points in total per histogram) versus a histogram of 100k samples conditioned on the same context points from the flow to get the overall shape, which is then re-normalized back to 10k overall counts. The x-y axes are omitted for a cleaner plot, but the histogram

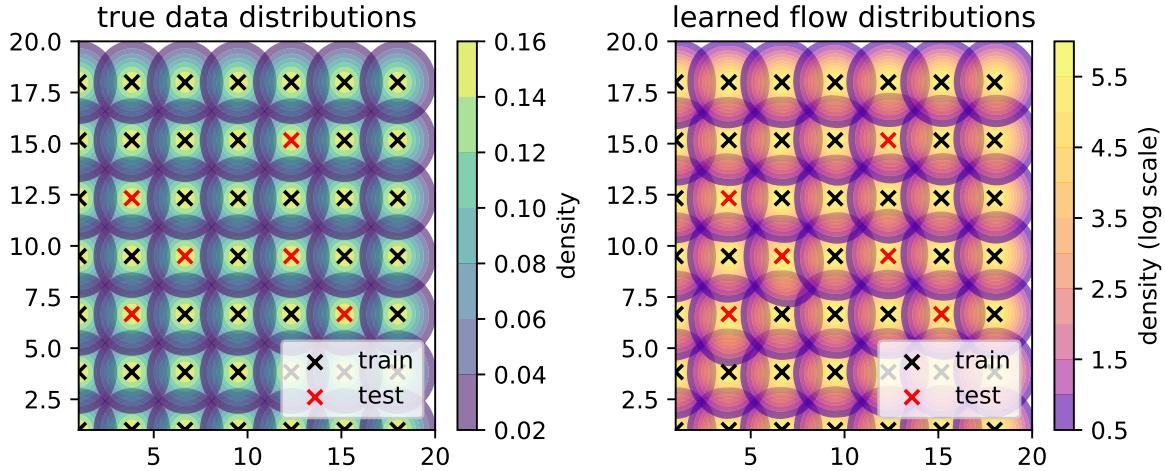


Figure 8.3: Left: the same grid of 49 different normal distributions from Figure 8.1. Right: the learned likelihood from the flow evaluated with context equal to the values of the means from the grid.

range is around ± 2.5 in each direction about the mean (imagine a square around one of the distributions in Figure 8.1).

The main thing we can get from this visualization is the imprint that subtracting the flow histogram from the data leaves. We can see this more prominently in Figure 8.5, where there are some biases left from the flow network getting the area around the mean slightly off. Green represents where the data counts are larger, and brown represents where the flow predicts larger counts. The scale of the colorbar in each case is worth noting – for a histogram of size 10k, these are relatively tame differences, but differences nonetheless (relative bin-wise differences would also be nice to view, but are inflated somewhat by small bin counts away from the mean).

8.3.4 Pulls

These plots are only half the story; we'd much rather see how the flow *uncertainties* affect these results. Instead of doing this bin-by-bin where small localized uncertainties make for difficult visualization, we plot the *pulls* aggregated over all training and test points separately. The pull here for one bin is defined as

$$\text{pull} = \frac{\text{flow prediction} - \text{data prediction}}{\sigma_{\text{flow}}} ,$$

where the uncertainty σ_{flow} comes from the standard deviation of the counts from the three histograms in that bin, which were produced by sampling each flow in turn. Without making

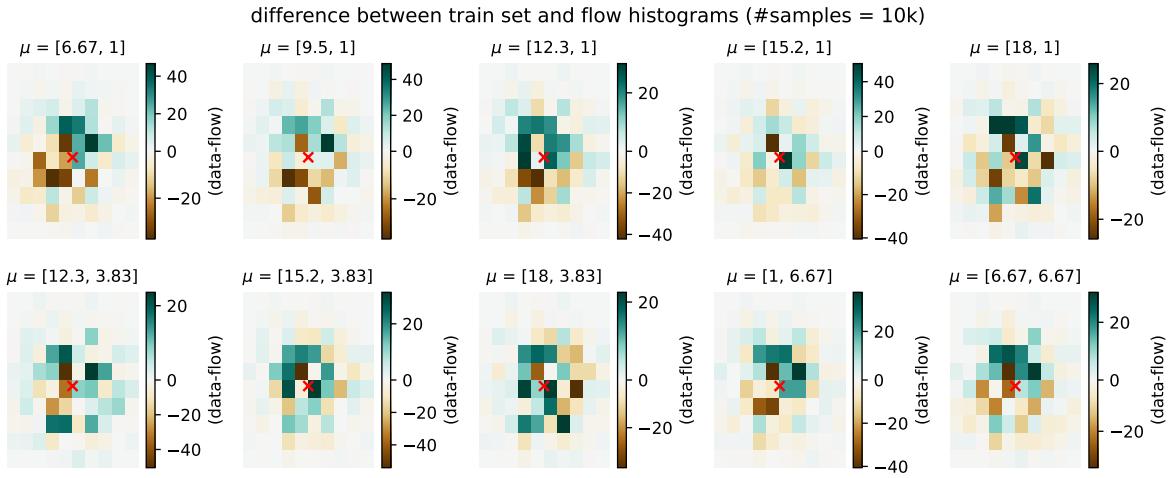


Figure 8.4: Differences between flow and data histograms across training context points, where each histogram is of 10k data points. The red cross marks the position of the mean of the true distribution.

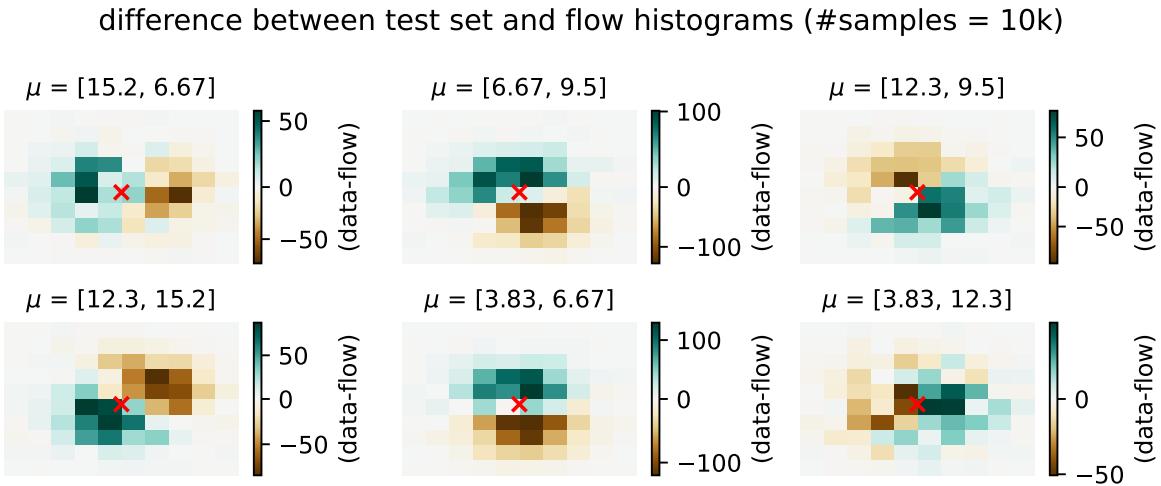


Figure 8.5: Differences between flow and data histograms across unseen, test set context points, where each histogram is of 10k data points. The red cross marks the position of the mean of the true distribution.

any strong theoretical claim, the reasoning to plot this quantity is to loosely follow the intuition behind the central limit theorem, where we assume that the bin counts will tend to a normal distribution in the limit of many repeated experiments. If the flow is a good predictor of the mean of that normal distribution, we'd observe the data being distributed as approximately $\text{Normal}(\text{flow}, \sigma_{\text{flow}})$. This ballpark statement is somewhat realized in Figure 8.6, where we plot histograms of the pull aggregated across all training contexts (left plot) and testing contexts (right plot).

The results are fairly unbiased in either case, with a spread of pulls being fitted a little wider than a standard normal. Beyond this, it's clear that if the error in the denominator is of comparable to the difference between data and flow, we're fairly happy that we know where we're wrong to some degree. Using this ensemble uncertainty is then a reasonable way to predict the failure modes of the flow for this simple example.

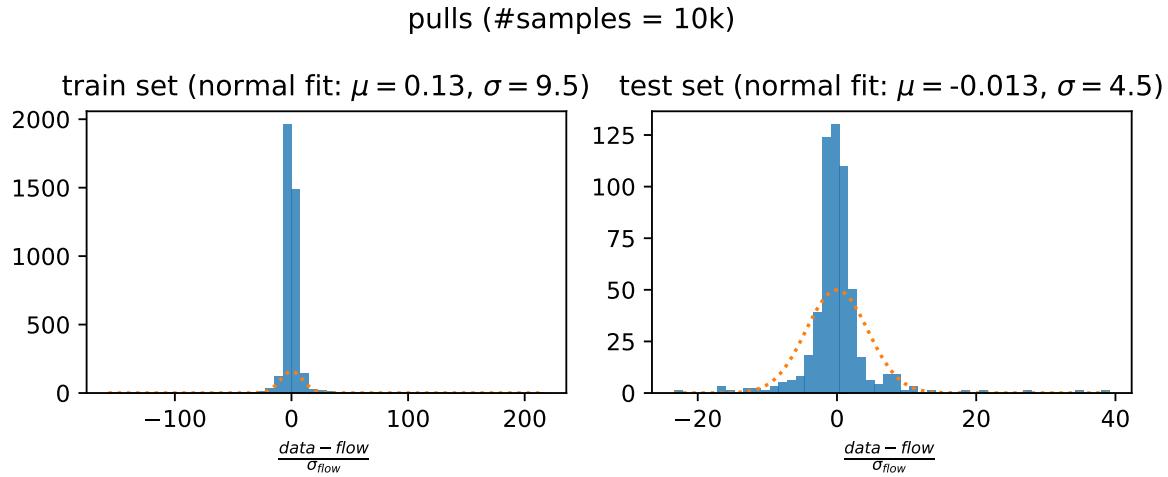


Figure 8.6: Plot of the pull for training contexts (left plot) and testing contexts (right plot). A fitted normal distribution is also shown for illustrative purposes.

8.4 Example 2: Gaussian firework

We now add a degree of complexity. Keeping with the theme of normal distributions, we'll let the mean influence the covariance matrix such that the distribution will rotate based on its position relative to the origin. More formally, for $\mu = [\mu_x, \mu_y]$, this parametrization $\text{Normal}(\mu, \Sigma)$ can be constructed by the following steps:

$$\theta = \arctan(\mu_y / \mu_x); \quad r = \sqrt{\mu_x^2 + \mu_y^2}$$

$$\Rightarrow \Sigma = MM^T, \text{ where } M = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} 1/r & 0 \\ 0 & 1 \end{bmatrix}. \quad (8.1)$$

This rather weird formula, found using inspiration from a blog post on a geometric interpretation of the covariance in a Gaussian (Spruyt 2014), applies a rotation and a scaling in proportion to the mean. By generating the same grid of points as in Figure 8.1, we end up with the result in Figure 8.7. I've affectionately termed it a Gaussian firework, since it makes a wonderful explosive pattern when plotted symmetrically about the origin, which I additionally show some examples of in Figure 8.10.

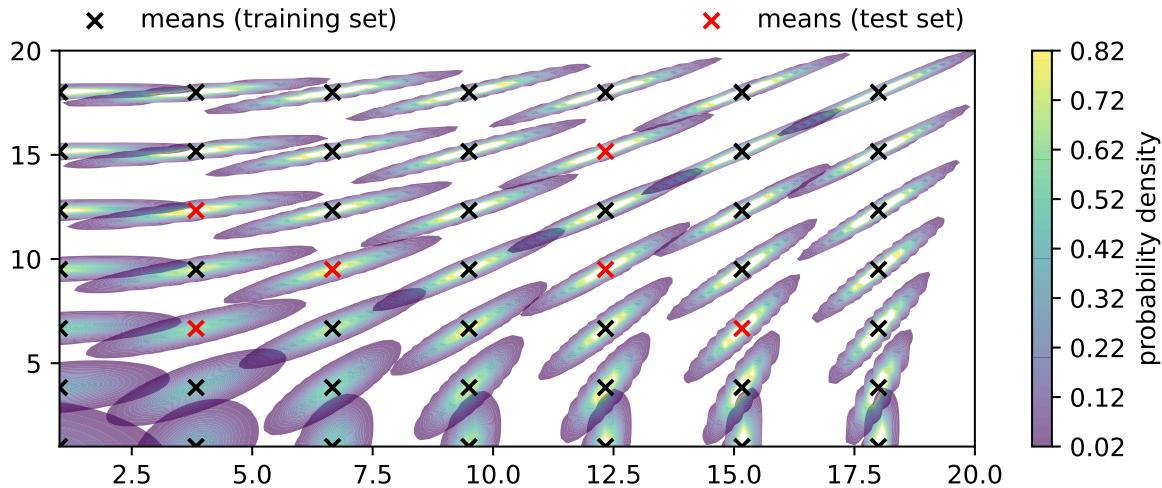


Figure 8.7: A grid of 49 different normal distributions, each with a mean corresponding to a cross on the image, and with covariance as defined by Equation 8.1. The contour representing 0 is omitted for visualization purposes.

Modelling this firework is more challenging for a couple reasons. The first is that we have some kind of symmetry of rotation that the flow needs to pick up on, using only information from the mean. The second is that the distributions are very tight about their means – a slight mis-guess will show a considerable error when making the same visualizations as in the simple example.

The hyperparameters for the training are the same as the previous example, including the points in the train/test sets, so we jump straight to the results.

8.4.1 Loss curves

See Figure 8.11 for a comparison of the negative log-likelihood loss for train and test sets. Again, this is just one of the three flows for illustrative purposes. We notice that the training

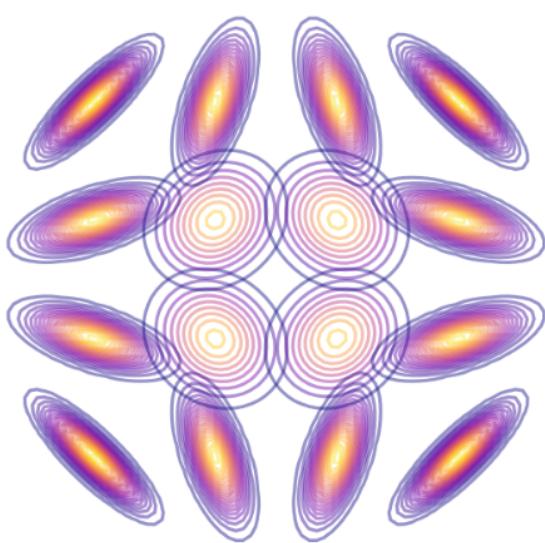


Figure 8.8: Some distributions plotted symmetrically about the origin.

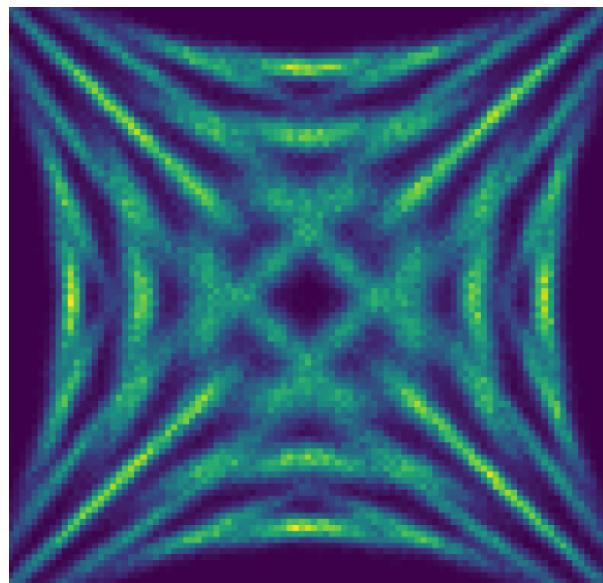


Figure 8.9: Histogram of many samples drawn from a grid of distributions about the origin.

Figure 8.10: A couple of fun plots to show the naming convention of “Gaussian firework”.

stops much earlier, which is due to the fact that the difference between train and test sets is much more significant here, with it being easier to overfit to the training samples alone.

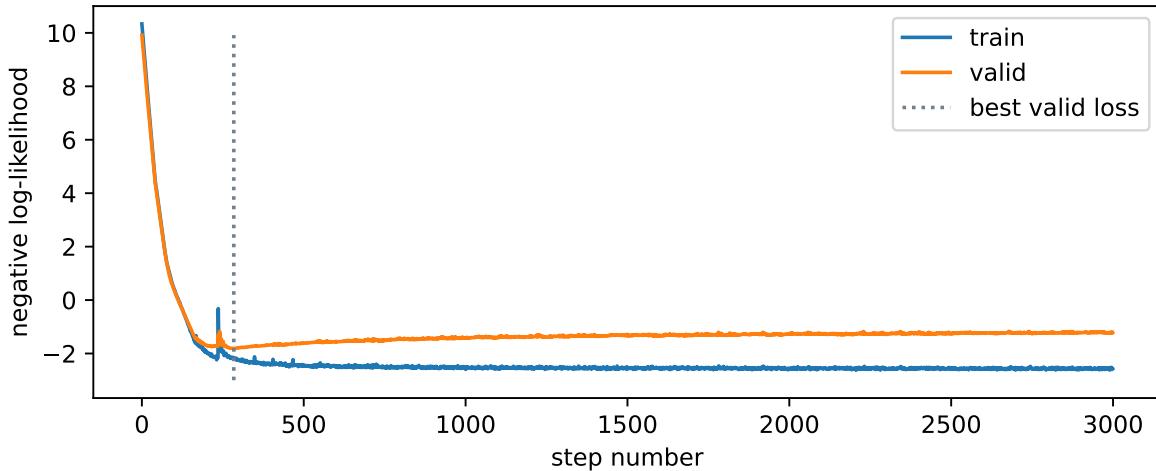


Figure 8.11: Example loss curves from a single flow trained on the Gaussian firework scenario. The model weights are extracted from the best test loss.

8.4.2 Distribution similarity

We can see the plots of the learned likelihoods from the flow ensemble in Figure 8.12. The topic of the scale difference is exacerbated further, which I'd guess is due to the concentrated nature of the distribution, allowing for the clustering of all the density in one place to quickly achieve a good loss for the training data.

We note the fairly good modelling of the way the distribution shape varies across the training points in particular. The shape of the distribution far from the mean at the unseen test set points (red crosses) is a little less well-modelled, with the mean being slightly off-center sometimes, and the contours not being as even.

8.4.3 Histogram similarity

Coming again to histograms, we do the same plots as for the first example, beginning with the raw differences in Figure 8.13 and Figure 8.14. The scale of the errors in the training set are equivalent to those in the simple example, but we see that the test errors have some vast differences by comparison. Since the distributions are so concentrated, you can effectively see the flow distribution in brown, and the data distribution in green for the test context points. This example is particularly unforgiving for the biases introduced as a result of the flow not having seen these points, since a slight mismodelling introduces a large error. Additionally,

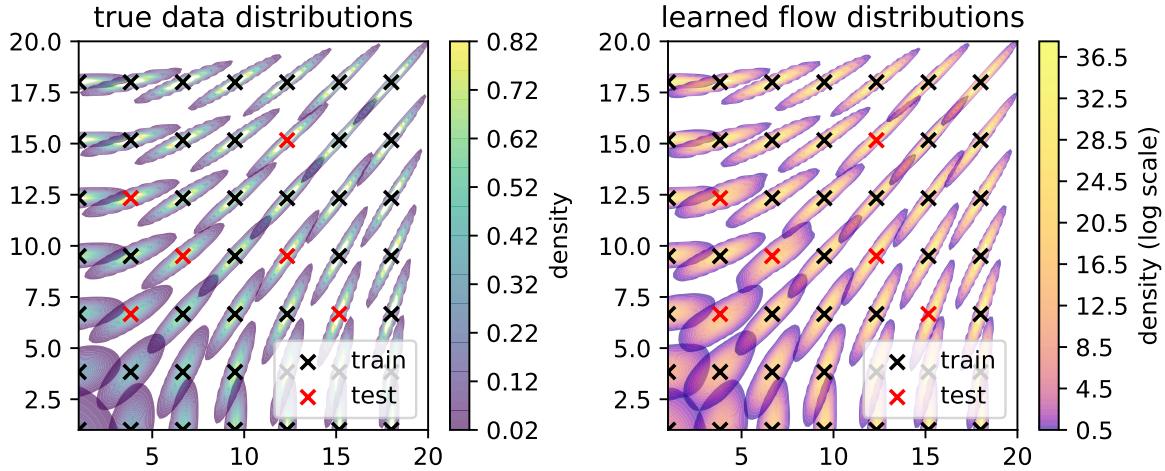


Figure 8.12: Left: the same grid of 49 different normal distributions from Figure 8.7. Right: the learned likelihood from the flow evaluated with context equal to the values of the means from the grid.

from a shape perspective, the centers are roughly coincident, but the rotation inferred from the context is a little different in most cases.

8.4.4 Pulls

Unlike in the simple example, the magnitude of the flow ensemble uncertainty is not great enough to save us in every case when we make the pull plots, which are shown in Figure 8.15. We see that the flow applied to the training distribution is reasonably unbiased in its prediction of the histogram counts, but the test set is far less forgiving – we have some points that are extremely far from 0, due to the flow difference being large and the uncertainty being comparably small.

8.5 Discussion

By and large, this method performed fairly well on the two toy examples it was tested on. It's clear that there is some very deliberate contextual inference, which is found from training in a way that conditions on the parameters that generated the samples, and generates a good proof of context for the viability of this method. This being said, there are definite shortcomings in the test set of the second example, which I'll address with my thoughts below, including how it's inherently linked to some of the training methodology decisions, and why I'm not overwhelmingly pessimistic about it.

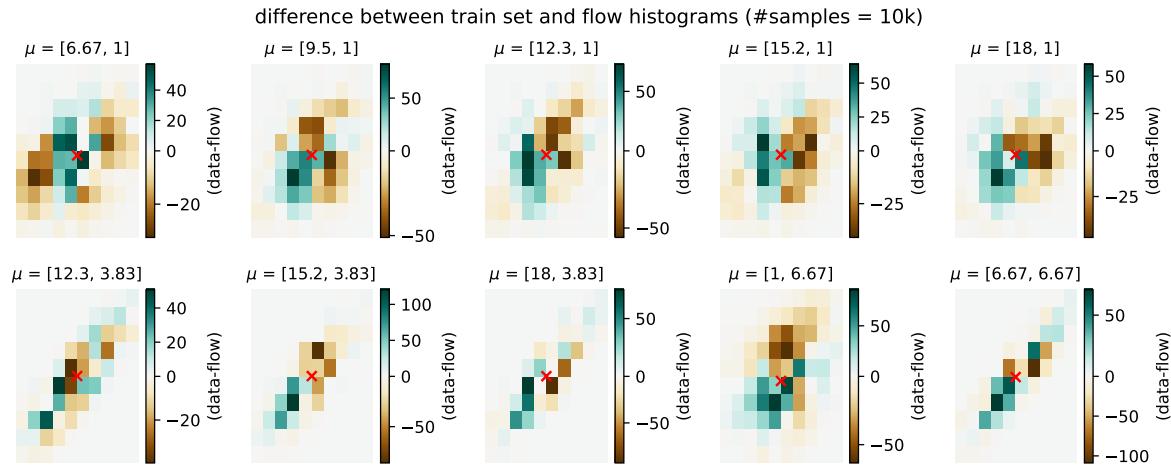


Figure 8.13: Differences between flow and data histograms across training context points for the Gaussian firework example, where each histogram is of 10k data points. The red cross marks the position of the mean of the true distribution.

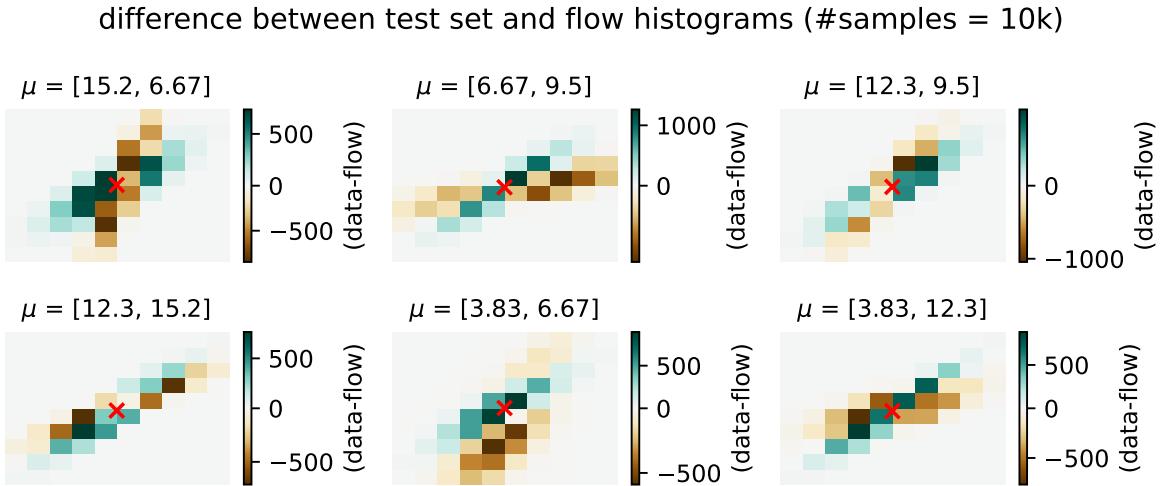


Figure 8.14: Differences between flow and data histograms across unseen, test set context points for the Gaussian firework example, where each histogram is of 10k data points. The red cross marks the position of the mean of the true distribution.

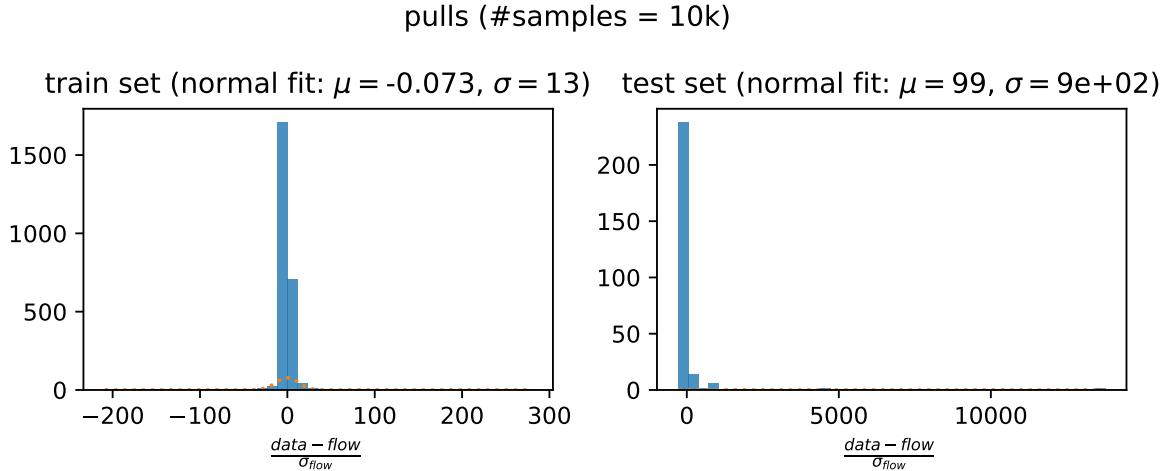


Figure 8.15: Plot of the pull for training contexts (left plot) and testing contexts (right plot) for the Gaussian firework example. A fitted normal distribution is also shown for illustrative purposes.

We can point at many things that could explain the interpolation failure modes in the second example: flow architectures that are too inflexible to model the very concentrated shapes, the limitation of training data points provided (both in number of data points and context grid density), not training with the best hyperparameters (no tuning was done), or perhaps the flow ensemble was too small.

8.5.1 What's the true “test set”?

Another reason for interpolation failures is that removing the test set points will fundamentally bias the model away from learning to generalize to the points we removed, when we technically had that information to learn from in the first place. This creates a paradox with assuming a train and test split – in what way should we do this? One could think of an example involving vital medical data, where it's essential to learn from the points provided instead of discounting large numbers of examples for validation.

One way to do this is to just do the train/test split in the *data* instead of in the *context*. That would be akin to more standard practice in traditional machine learning, for instance, but neglects keeping a good measure of the interpolation performance. As mentioned previously, there was a notion of a “valid” set that was played with during the examples that does this to some extent already by holding out a small fraction of data from training context points. However, if we did this for *all* context points, we'd have to blindly trust the flow uncertainty to account for the predictive uncertainty to new points. One could perhaps do some k-fold or leave-one-out cross validation, where the model's generalization ability could be conservatively

quantified by training multiple flows on data with one context point removed, repeating this across all points in the interpolation regime, and quote the ensemble uncertainty or the predicted vs actual error for each of these cases as a better idea of the predictive uncertainty. A caveat to this is that these models are all different to the one that actually would be used in practice, and there would have to also be some kind of secondary interpolation/extrapolation mechanism to produce this cross-validation uncertainty in a continuous way across the context space. These ideas were not tried due to time constraints, but could be the subject of further work.

In the next section, we'll re-use this method, but we'll also compare it to statistical uncertainties in the histograms themselves, and see if we do better than just the predictive uncertainty on the flow (not here purely due to time).

9 Search for a heavy scalar particle X decaying to a scalar S and a Higgs boson, with final state $b\bar{b}\gamma\gamma$ in the ATLAS detector

As part of my PhD, I made some various contributions to a search for a physics process $X \rightarrow SH \rightarrow b\bar{b}\gamma\gamma$, where X and S are scalar particles beyond the Standard Model. My contributions include:

- building a faster framework for data processing
- assisting with the development of a pipeline to classify signal versus background using a neural network parametrized in the truth-level masses m_X and m_S
- using the method I developed with normalizing flows to interpolate a 2-D signal shape across different signal mass points
- various small contributions to the statistical analysis setup
- the proposal of a new observable based on normalizing flows

The analysis of this data is still in the preliminary stages at the time of writing, so take all these studies with a grain of salt.

Also, a quick note on shorthand for this section – you’ll see me write notation like $H(bb)$ – this means that we’re looking at the case where a Higgs boson is decaying to two b -quarks as its final state.

9.1 Overview and motivation

The new particle discovered in 2012 (ATLAS-Collaboration 2012) is widely regarded to represent the Higgs boson as predicted by the Standard Model, which is predicted to have a rest mass of 125 GeV. While this is confirmatory of the existence of some flavor of the Standard Model, we know this isn’t the end of the story. Many physics theories beyond the Standard Model predict some kind of Higgs sector, where additional scalar bosons could exist and interact with the Higgs in some way, but have yet to be discovered. To this effect, it is useful to probe data taken from proton-proton collisions to see if particles produce states that correspond to e.g. resonances that look like these new scalars.

In particular, this work looks at the process $X \rightarrow SH \rightarrow b\bar{b}\gamma\gamma$, where X is a heavy scalar with a mass large enough to produce a Higgs with Standard Model mass (i.e. $m_H = 125$ GeV) and a scalar S with mass m_S such that $m_X > m_S + m_H$, which makes the decay $X \rightarrow SH$ satisfy energy conservation. I found an example for something that looks like a candidate event for this process as-seen by the ATLAS detector, shown in Figure 9.3.

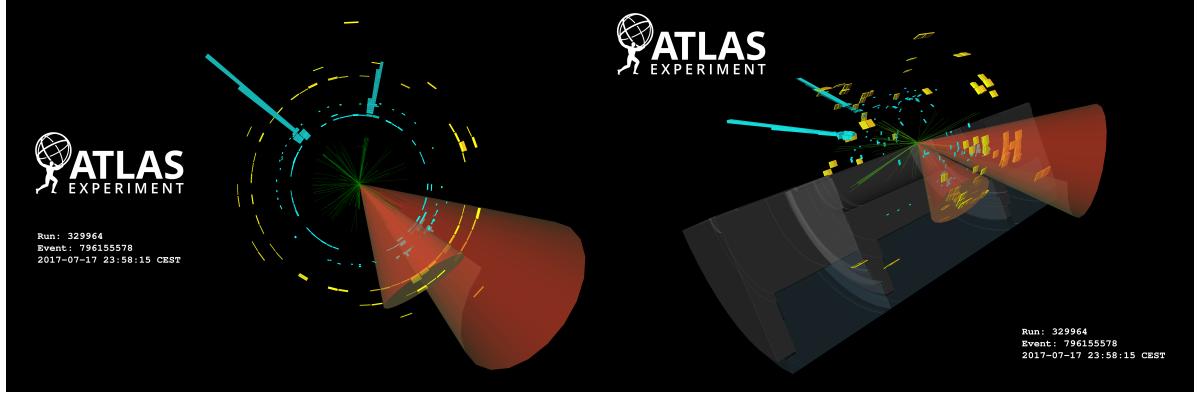


Figure 9.1: Cross-sectional view.

Figure 9.2: 3-D view for depth.

Figure 9.3: An example of a event's wake in the ATLAS detector, which looks very similar to that we would see from $X \rightarrow SH \rightarrow b\bar{b}\gamma\gamma$, where there are two blue lines that the photons leave as a signature, and two cones from the b -jets. Attribution: (Aad et al. 2022).

This particular process is predicted by a number of different theories, including but not limited to:

- Next-to-Minimal two-Higgs Doublet Model (He et al. 2009)
- Next-to-Minimal Supersymmetric Standard Model (Ellwanger, Hugonie, and Teixeira 2010)
- Complex two-Higgs Doublet Model (Ilya F. Ginzburg, Maria Krawczyk and Per Osland 2002)
- Two-Real-Scalar Standard Model extension (Tania Robens and Wittbrodt 2020)

It's worth noting the problems that these theories solve (i.e. why they are interesting at all), which span combatting matter-antimatter asymmetry mechanisms in the early universe (Jiang et al. (2016)) to producing possible dark matter candidates (Gonderinger, Lim, and Ramsey-Musolf (2012)) amongst other things. Recall our discussion in Section 1.4 that went over some extra issues of this nature, e.g. the hierarchy problem.

The next thing to address is why it's worth it to look at $b\bar{b}\gamma\gamma$ as a final state. The first reason is that if we assign the di-photon state as originating from a Higgs boson, we would have a very clear way to select events we want to analyze, as experiments at the Large Hadron Collider have the ability to precisely determine the energies of photons in their electromagnetic

calorimeters. Events originating from decays of interest would then leave a fairly sharp peak at 125 GeV in the invariant mass spectrum of the two-photon system, which we can turn into a requirement for including those events in our analysis. This would leave the b quarks (which would be seen in the detector as jets due to hadronization) as originating from the S particle, which is the dominant decay mode of the S when one assumes that it has properties similar to the Standard Model Higgs. Of course, despite all this, choosing any one particular final state is a needle-in-a-high-dimensional-haystack approach, with there being many other choices of theories and states to consider. In that sense, there is no particular reason other than to look where has not been checked yet.

What exactly are we looking for then? As alluded to in Section 3.3, searches for new particles involve calculating p -values (or CL_s values), either trying to reject a background-only hypothesis for discovery, or to set an upper limit on the signal strength. We concentrate on the latter, with the steps ahead demonstrating the task of the analyzer to optimize the workflow for this purpose.

9.2 Simulated data

Data for the signal process of $X \rightarrow SH \rightarrow b\bar{b}\gamma\gamma$, where the b quarks are associated to the S and the photons are associated to the Higgs boson, was generated at a variety of possible combinations of m_X and m_S . We can see the points chosen in Figure 9.4, where the upper-left quadrant is kinematically forbidden (there, $m_X < m_S + m_H$). Sensitivity to this process is forecast to be reasonable up to around $m_X \approx 900$ GeV and $m_S \approx 300$ GeV (by (Sebastian Baum, Nausheen R. Shah 2010)), which we conservatively extended to 1000 GeV and 500 GeV respectively. We began with just the grid on the bottom-left, and later extended this sparsely to the high mass region.

The different specific event generator tools used for all of the simulation were PYTHIA (Sjöstrand et al. 2015), SHERPA (Bothmann et al. 2019), EvtGen (Ryd et al. 2005), and NNPDF (Ball et al. 2015). We can segment their use for the two cases for signal and background.

For signal processes, samples were generated for each mass point in Figure 9.4 at leading order (i.e. only the simplest processes for that interaction) with Pythia 8 doing the underlying quantum field theory calculations. EvtGen was used to simulate the fragmentation of the b -quark jets into hadrons. NNPDF 2.3 controlled the set of parton distribution functions used, which dictate the interior structure of the protons that are colliding, and therefore play an important role in the calculations for different scattering probabilities when the constituents of those protons collide. Additionally, there are effects It's worth mentioning that the new scalar particles X and S were generated using what's called the *narrow-width approximation*, which simplifies calculations greatly by assuming the particles are very short-lived before decaying, and results in more narrow invariant mass spectra as a result.

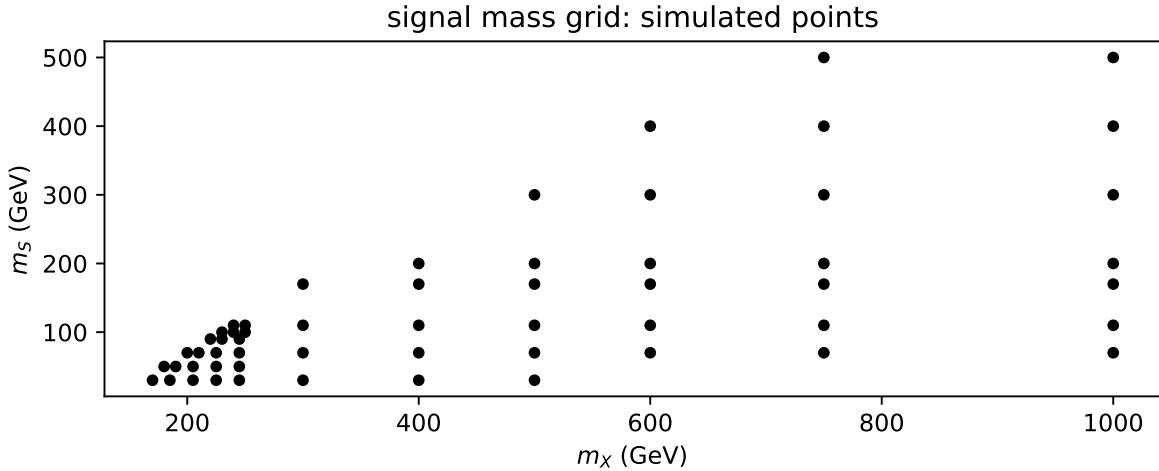


Figure 9.4: A grid of the different points for which data originating from the signal process was simulated.

In the case of background – that is, every Standard Model process that could possibly generate a final state of two b quarks and two photons – things get a lot more complicated, since there are many more processes we need to consider. To add more granularity to this, the main contributions that were simulated include:

- Interactions involving the strong force (known as QCD, or quantum chromodynamics) that result in two photons and two jets (shorthand $\gamma\gamma jj$)
- Associated production of a Higgs boson and two top quarks ($t\bar{t}(bb)H(\gamma\gamma)$)
- Fusion of two gluons to a Higgs, where a gluon in the process fragments to a bb pair of jets (ggH)
- Associated production of a Z boson and a Higgs, where the Z decays hadronically to quarks ($Z(qq)H(\gamma\gamma)$)
- Different types of di-Higgs events, where two Higgs bosons are produced

Despite this separation, when event weights are produced, the $\gamma\gamma jj$ background completely dominates all the others (> 99% of the contribution to the total event weights). The different simulation contributions are summarized in Table 9.1 for those that want more detail, but it's worth noting that the methods I worked on treat the background sample as one unit, equal to the concatenation of all events from these processes, which is an intentional simplification.

Table 9.1: Different simulation tools used for the individual background processes.

Process Type	Physics simulators	Parton distributions (Probabilities)	Parton distributions (Showering)	Production Mode
Single Higgs	NNLOPS + PYTHIA8	PDFLHC	AZNLOCTEQ6 ggH	
Single Higgs	POWHEG + PYTHIA8	PDFLHC	AZNLOCTEQ6Vector-boson fusion	
Single Higgs	POWHEG + PYTHIA8	PDFLHC	AZNLOCTEQ6 V^+H	
Single Higgs	POWHEG + PYTHIA8	PDFLHC	AZNLOCTEQ6 V^-H	
Single Higgs	POWHEG + PYTHIA8	PDFLHC	AZNLOCTEQ6 $q\bar{q} \rightarrow ZH$	
Single Higgs	POWHEG + PYTHIA8	PDFLHC	AZNLOCTEQ6 $gg \rightarrow ZH$	
Single Higgs	POWHEG + PYTHIA8	PDFLHC	A14NNPDF23 $t\bar{t}H$	
Single Higgs	POWHEG + PYTHIA8	PDFLHC	A14NNPDF23 bbH	
Single Higgs	MGMCatNLO + PYTHIA8	NNPDF	A14NNPDF23 $tHbj$	
Single Higgs	MGMCatNLO + PYTHIA8	NNPDF	A14NNPDF23 tHW	
di-Higgs	POWHEG + PYTHIA8	PDFLHC	A14NNPDF23 $ggHH$	
di-Higgs	MGMCatNLO + PYTHIA8	NNPDF	A14NNPDF23 VBF HH without VHH	
QCD	SHERPA2	SHERPA2	SHERPA2	$\gamma\gamma + \text{jets}$ (0-4), $m_{\gamma\gamma} \in 90 - 175 \text{ GeV}$
QCD	MGMCatNLO + PYTHIA8	MGMCatNLO	MGMCatNLO	$t\bar{t}\gamma\gamma$

9.3 Preprocessing and selection

Before analyzing the data we simulated above, which gives us access to kinematic quantities of the objects in the detector, there is typically a pre-filtering stage – called a **preselection** – where we slim down this dataset to only things that we’re interested in based on a set of

criteria. To talk about that, we'll have to first speak a little about jets, which need a bit more work due to their very messy signature from all the showering into hadrons.

9.3.1 Tagging b -jets

Just as a reminder, quarks are never seen alone – they're always in some composite state with other quarks, which we call hadrons. When a quark is produced in a decay, it will really be bound somehow to a different quark, which we can picture as a rope. When the rope breaks from them going too far away, we can think of each end of the rope turning into a new quark to keep the state stable. We call this **hadronization**, and it's this process happening over and over again that forms a spray of particles that has a conic shape, which we call a jet.

Now, how might we distinguish a jet that comes from two different quark types? There aren't any particularly clear differences from first principles that I know of, but since quarks differ in concrete ways (mass being the main one), we'd expect the jets to have subtly differing dynamics. That's why we need more complicated algorithmic systems to tell these jets apart based on their properties, which are colloquially called *taggers* since they tag a jet with a label of the quark type. Taggers are usually something like a neural network, which can take in many different inputs about the structure of the jet, and give us a single number that represents the likelihood of that jet being of a certain type. Since the Higgs boson most commonly decays to two b -jets, we have very specialized b -taggers in particle physics. We're very interested in making use of these b -taggers to help us identify which jets in our events came from b -quarks, which could sign our scalar S .

The way this appears to the analyzer is that each jet object in our data will have a score that the b -tagger has given the jet based on its properties. (working point)

9.3.2 Selection for this work

There are many different analyses selections being trialed at the time of writing; the results that follow are all performed with a simple “loose” criteria imposed on the data, which requires:

- at least two selected photons
- no leptons
- at least 2 central jets (central = originating from the main collision center, or *primary vertex*)
- less than 6 central jets
- at least one jet above the 70% working point threshold for b -tagging
- less than 3 b -tagged jets at the 77% working point

We also accept any data with exactly 2 b -jets at the 77% working point threshold, as this will likely allow us to reconstruct the invariant mass m_{bb} well – something very important if we want to precisely determine if our events peak at the mass of our new scalar S .

9.4 Fit strategies

A few strategies were investigated to see which variables provided the most discriminating power when comparing their distribution in signal and in background. The reason for this is that we want to pick a *summary statistic* of the data to use as a foundation for the HistFactory statistical model construction (Section 3.2), and choosing something that differs in a significant way across signal and background distributions should hopefully give us smaller p -values and stronger limits.

We go over the two main approaches explored in the following sections.

9.4.1 2-D fit in the $m_{bb\gamma\gamma}$ and m_{bb} plane

A somewhat natural choice to look at is the variables that, when constructed, recover the mass resonance for each of the proposed new particles X and S . We thus look at the invariant mass of the overall final state $m_{bb\gamma\gamma}$ (which should peak at the chosen value of X) and the invariant mass of the b -tagged jets m_{bb} (which should peak at the chosen value of S). Some example plots for the shape of these distributions in the signal and background Monte-Carlo samples can be found in Figure 9.7.

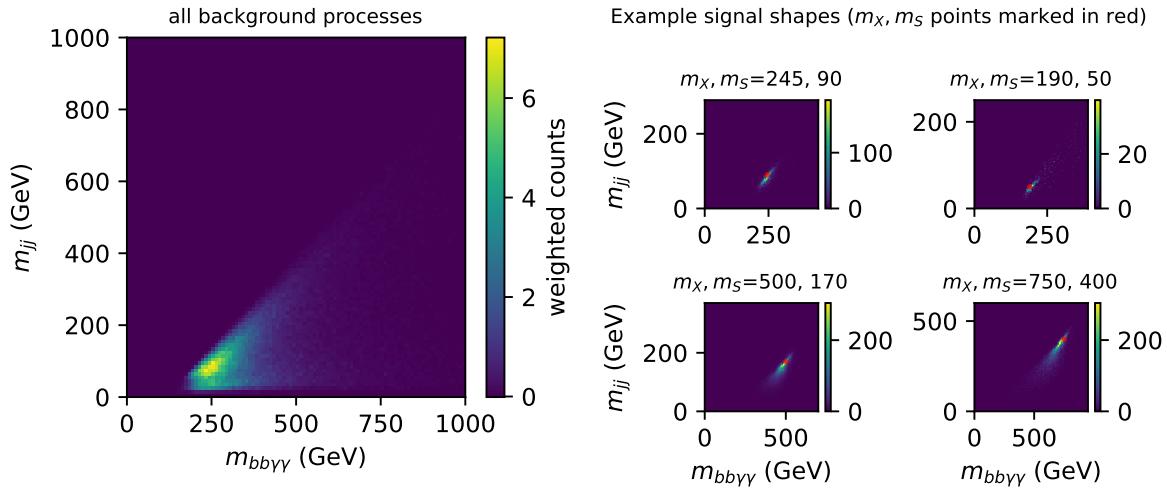


Figure 9.5: Total background shape.

Figure 9.6: Some example signal shapes.

Figure 9.7: Some example distributions of the $m_{bb\gamma\gamma}$ and m_{bb} invariant mass plane.

9.4.2 1-D fit using a parametrized neural network-based summary statistic

You may have thought based on earlier discussion that it may not be the case that a one-size-fits-all variable (or variables) exists across every combination of m_X and m_S featured in Figure 9.4, or indeed across any possible combination of hypothesized masses. It is then of interest to look for an observable that can be *parametrized* in the truth masses m_X and m_S such that the chosen observable can adapt to provide better results depending on the hypothesis we're probing. An example of such an observable is the so-called **parametrized neural network** (pNN), originally proposed in Baldi et al. (2016).

We're interested in neural networks more generally for their ability to provide flexible outputs (here, 1-D) that can learn to perform as we train them to do so, e.g. to discriminate strongly between events coming from signal and background respectively. The way a pNN is structured is no different to that of any other neural network, with the only change being the inclusion of the parameters of your physics model (here, m_X and m_S) as additional inputs. This aims to essentially use those inputs as choosing the best model for the use case; when comparing different values of the inputs, the information from one set of values will likely be propagated through the network in a very different way to the other set, which can provide information about the context in which the network is performing inference in. Training a pNN is then no different to standard procedures – by providing the additional inputs within a batch, the loss structure of choice doesn't have to change in any way to accommodate this, but will optimize for good average performance across all provided contexts. Moreover, if the network is able to infer this context well from the provided physics parameters, the performance of the network should carry over to new, unseen parameter points (which for us would be the gaps between the points in Figure 9.4).

Practical training considerations

When training this model for our use case, a number of practical issues arose. The first is that we need to provide a set of signal truth masses for *all* events, including those coming from background. Of course, these labels do not exist; following the approach in Baldi et al. (2016), we then circumvented this to some degree by uniformly sampling these labels from the distribution present in the signal events, and assigning these as the labels to background events. The rationale behind this is to try and encode as little additional information as possible, hoping that the network will still be able to pick up the distribution of the signal context instead. Another issue is that of scaling the input variables, with it being common practice to scale all inputs to either reside in the range [0,1], or to have zero mean and unit variance. This scaling also needs to be applied to the truth masses; depending on the method chosen, the distribution of the masses could become very skewed to 0, which has the potential to make it more difficult to encode the context information for having very low values numerically.

Many combinations of input variables were tried, with some examples being kinematics like p_T , η , ϕ (for the 2 photons and the 2 jets with highest p_T), differences in these variables such as

$\Delta\phi(\gamma_1, \gamma_2)$, $\Delta\eta(\gamma_1, \gamma_2)$, and also non-linear quantities like the angular distance between objects $\Delta R = \sqrt{\Delta\phi + \Delta\eta}$. Despite all this, the most effective training input configuration was found to just be using only the invariant masses $m_{bb\gamma\gamma}$ and m_{bb} , which speaks to the power of the 2-D fit approach previously mentioned. An example pNN output for one of the signal points (evaluated on unseen test data only) can be found in Figure 9.8, created by my collaborator Laura Pereira Sánchez, who spearheads this work.

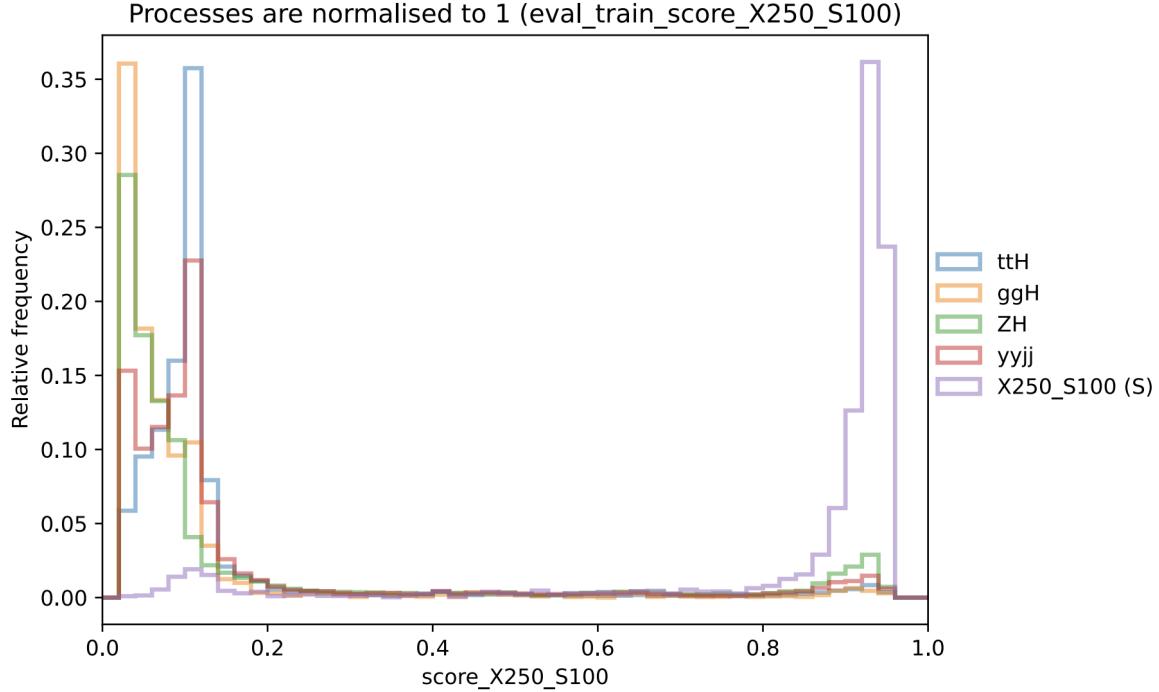


Figure 9.8: Example pNN showing discriminating power post-training when conditioned on the signal point $m_X = 250$ GeV, $m_S = 100$ GeV. (Attribution: Laura Pereira Sánchez, Stockholm University)

9.5 Interpolation between signal shapes

For either strategy in Section 9.4, we're interested in some kind of way to make inference about points in-between those we've already simulated in Figure 9.4. We would of course like to just simulate points on the fly for any hypothesis we want to probe, but that's time, compute, and CO₂ that we'd rather not have in excess. In order to do this simulation-free, we need to produce the expected shape of the counts from simulation of that signal process. We're now in the regime of somehow trying to *interpolate* the shape of the signal in whatever variables we want to use as input to the HistFactory model. Moreover, it would be great if this could come

with a notion of uncertainty; by adding this uncertainty to our statistical model, we'll be able to quantify the fact that we're going to have a worse result in the regions for which we didn't simulate data directly.

This is exactly the context in which I developed the method presented in Chapter 8! I use **normalizing flows** that are conditioned on the truth masses m_X and m_S as a mechanism to interpolate between the signal shapes used for fitting. While this was initially designed as a strategy for the 2-D fit of $m_{bb\gamma\gamma}$ and m_{bb} , where samples from the flow would be drawn from the joint conditional distribution $p(m_{bb\gamma\gamma} m_{bb} | m_X, m_S)$ and histograms of those samples made for use as 2-D templates, the method works equally well for the 1-D pNN strategy. The reason for this is that we can just draw samples in the same way, and then build up the shape of the pNN output by computing the results given the flow samples, since the flow is defined over the same set of input variables $m_{bb\gamma\gamma}$ and m_{bb} . The resulting interpolation uncertainty can be found from averaging the yields from the 5 sets of samples, and the uncertainty from their standard deviation. We can then normalize this histogram to the appropriate amount, provided we have access to that factor (more on that later; we have to interpolate that too).

Exactly like in Chapter 8, a train/test split is made across a number of (m_X, m_S) points, which can be seen in Figure 9.9. Here, we don't make any separate valid split that involves the training grid data.

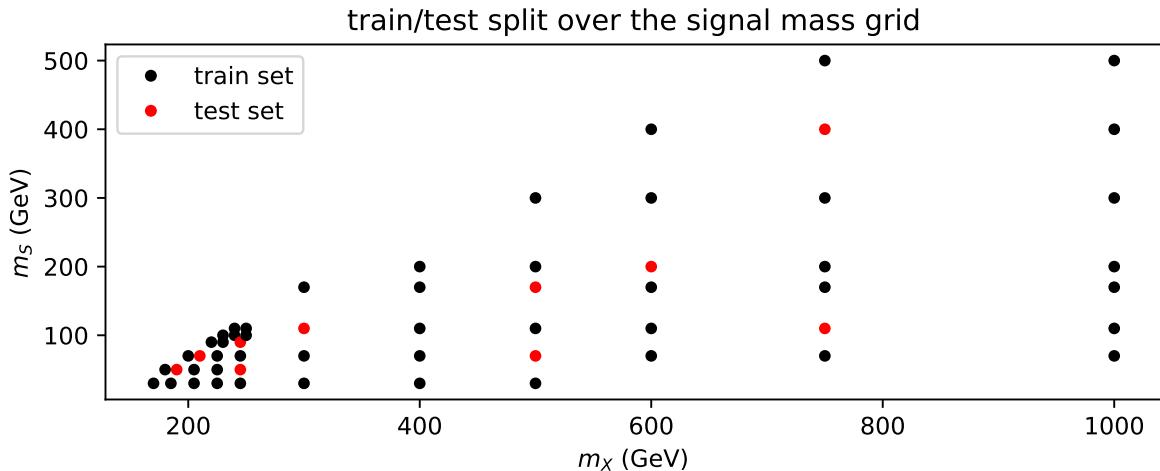


Figure 9.9: The train/test split across the grid of the different points for which signal process data was simulated.

The training setup is then to look at event-wise pairs of $m_{bb\gamma\gamma}$ and m_{bb} , along with the context label (m_X, m_S) representing the parameters at which the event was generated. These will be provided in batches, and used as input to the flow, which assesses its quality though calculating the mean negative log-likelihood across the batch, and then uses the gradient of this to update it's transform parameters. The results from this training procedure are the continuously defined

conditional distribution $p(m_{bb\gamma\gamma} m_{bb} | m_X, m_S)$, as well as the ability to draw samples from this distribution.

One practical aspect of this training procedure that I didn't cover in Chapter 8 is that of *event weights*. When applying this problem to a particle physics context, we're conscious of the fact that events are not supplied alone, but also with a weight that controls its relevance as a proportion of the distributions defined by that physics process. This means that the distributions we're trying to imitate with the flow need to be appropriately scaled according to these weights. A fairly simple way to do this is to just weight the contribution to the loss from a given event proportional to it's event weight, i.e. *multiply the loss of an event (the negative log-likelihood) by its weight*. The intuition behind this is that one would expect an event with weight 2 to have the contribution to the distribution of two individual events with identical $m_{bb\gamma\gamma}$ and m_{bb} values. It follows that the loss expected from those two events is just two equal contributions of loss at the same values of $m_{bb\gamma\gamma}$ and m_{bb} .

9.5.1 Results

I performed the training procedure as described for 5 flows with different initializations, and use their ensemble as the predictive model, with the standard deviations of these predictions (for likelihood values or histogram yields) acting as an uncertainty. The hyperparameters of the training procedure are very similar to the work in Chapter 8:

- Batch size of 4000 points
- 8 layers of linear, autoregressive transforms
 - Each transform's neural network has one hidden layer of 16 neurons
- Adam optimizer with a learning rate of 1e-3
- 10000 iterations total (from which the best performing iteration on the test set is selected).

We'll start by looking at the *binwise pull values* just as in Chapter 8, i.e.

$$\text{pull} = \frac{\text{flow prediction} - \text{data prediction}}{\sigma_{\text{flow}}} . \quad (9.1)$$

Figure 9.10 shows histograms of the pull accumulated over all training and test points separately, where the 2-D histograms of the pull in the $m_{bb\gamma\gamma}$ and m_{bb} plane are aggregated for each category of point. There's also a thresholding condition on these histograms such that the data doesn't predict less than 10 events in any given bin, else we could artificially inflate the performance of the flow when it's good at predicting values far from the bulk of the distribution. We notice that the performance on the test set has both a larger bias and variance due to the presence of some very large biases for a few of the test points. It's then of course interesting to investigate which points are the most problematic. We can visualize this through coloring each point on the signal mass grid with it's corresponding mean and standard deviation, which we do in

Figure 9.11. Here, it's clear that there are a few test points that are particularly problematic (strong pink coloring on both plots).

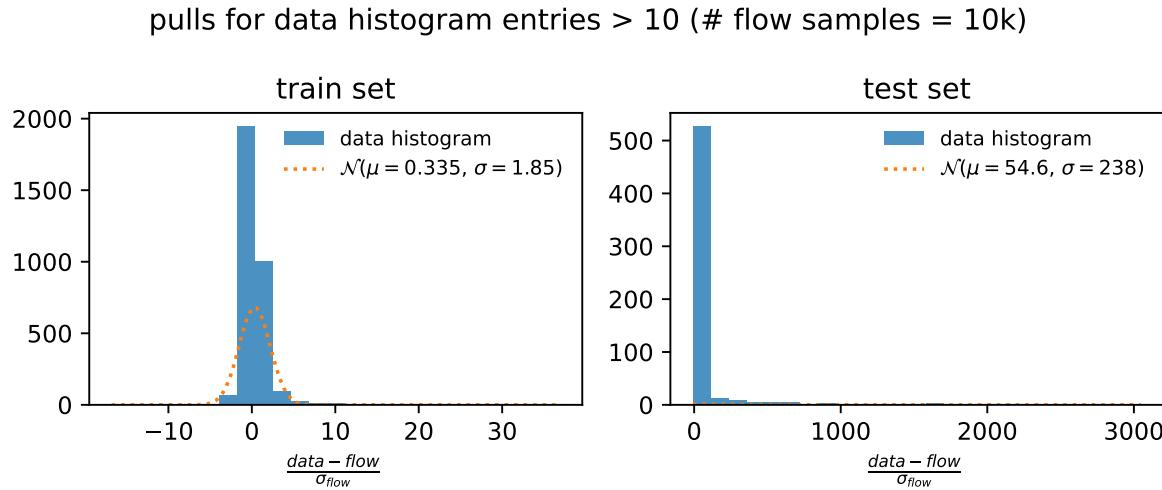


Figure 9.10: Left: Histogram of the bin-by-bin pull (using the flow ensemble uncertainty) accumulated across different context points from the training set. Right: Same for the test set. Both plots have a normal distribution fit overlaid.

Before advancing the discussion further, it's worth touching on another possible source of uncertainty. If we treat each bin count from simulation as the expected number of events λ for a Poisson distribution (as is done when modelling real data using HistFactory), we know that those shapes look remarkably like normal distributions of width $\sqrt{\lambda}$ for $\lambda \geq 10$ (see Section 2.1.6.2). The square root of the bin count then serves as a notion of so-called **statistical uncertainty** – a standard deviation's worth of room in which the actual count may differ from that predicted by simulation, purely from how many events lie in that bin¹. We can then do the same method as above, but replace the flow ensemble uncertainty with the square root of the bin count. These plots are shown in Figure 9.12 and Figure 9.13. We see a dramatic improvement in the test set! It would appear that while there are definitely distinct differences between flow predictions and data (a bias clearly still exists on the right), those differences are often within statistical uncertainties.

We can repeat this exercise one more time: instead of choosing one of these two uncertainties, we can just look at the maximum of either one in any given bin to attempt to cover us in the worst case scenario. Those plots are found in

¹in HEP-speak, high numbers of events = “high statistics”, hence the name

Distribution of the normal fit to the pull across the signal grid (σ_{flow} only)

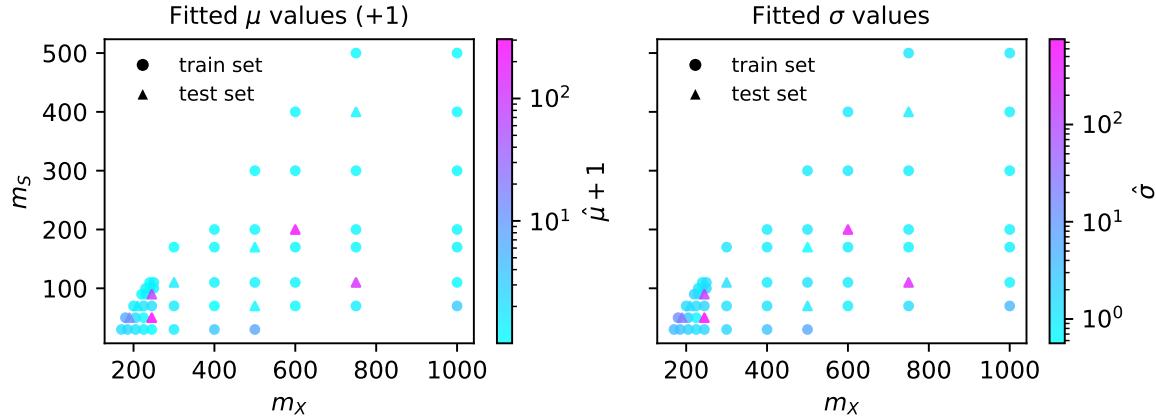


Figure 9.11: Left: Signal grid points colored by the mean of the pulls (using the flow ensemble uncertainty) for that point. Right: Signal grid points colored by the standard deviation of the pulls for that point.

pulls with statistical uncertainty for data histogram entries > 10 (# flow samples = 10k)

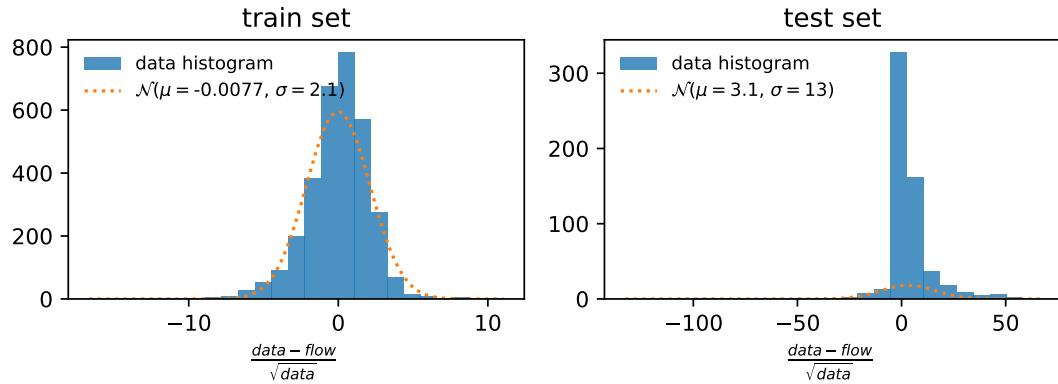


Figure 9.12: Left: Histogram of the bin-by-bin pull (using the statistical uncertainty only) accumulated across different context points from the training set. Right: Same for the test set. Both plots have a normal distribution fit overlaid.

Distribution of the normal fit to the pull across the signal grid (stat uncert only)

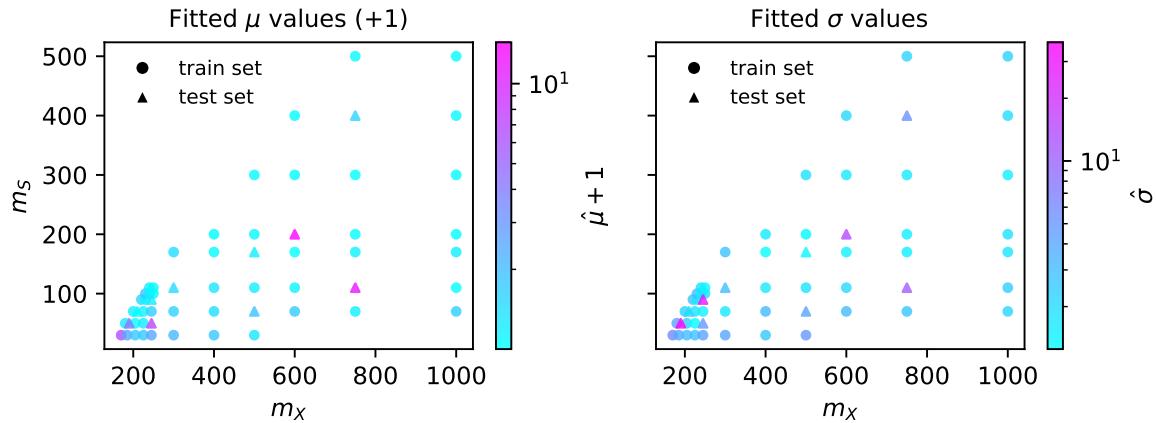


Figure 9.13: Left: Signal grid points colored by the mean of the pulls (using the statistical uncertainty only) for that point. Right: Signal grid points colored by the standard deviation of the pulls for that point.

pulls with both uncertainties for data histogram entries > 10 (# flow samples = 10k)

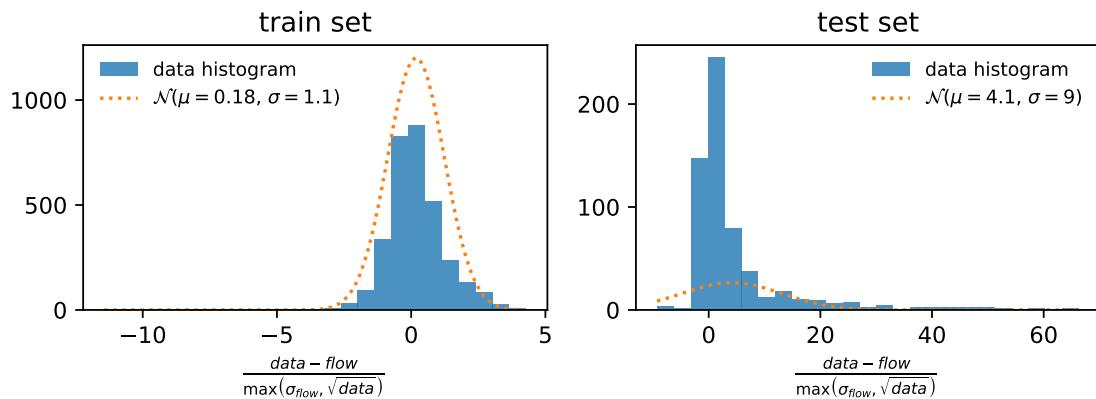


Figure 9.14: Left: Histogram of the bin-by-bin pull (using both the statistical and the flow uncertainty) accumulated across different context points from the training set. Right: Same for the test set. Both plots have a normal distribution fit overlaid.

Distribution of the normal fit to the pull across the signal grid (max[stat uncert, σ_{flow}])

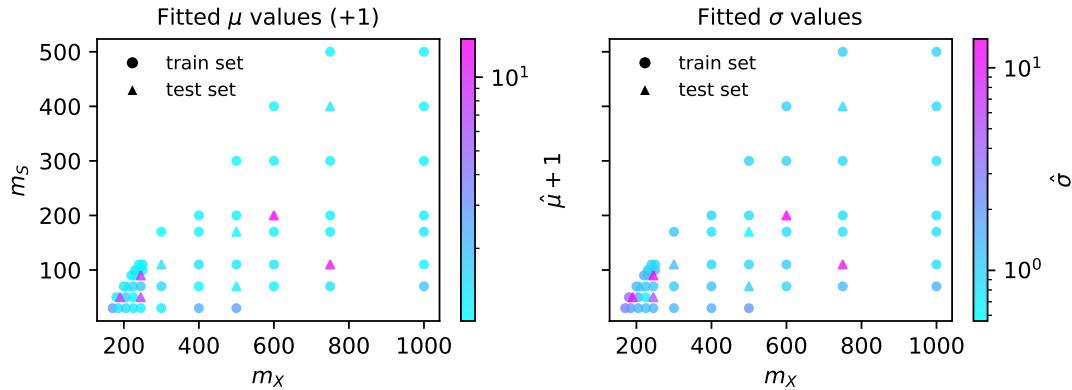


Figure 9.15: Left: Signal grid points colored by the mean of the pulls (using both the statistical and the flow uncertainty) for that point. Right: Signal grid points colored by the standard deviation of the pulls for that point.

9.5.2 Discussion

Overall, the flow training here shows clear signs of the ability to interpolate the signal shapes. In terms of criticisms, many of the relevant points from Section 8.5 apply here too, including not using any more advanced flow model, and the significant fact that we're restricting our ability to interpolate by holding out information in what is an inherently sparse feature space. The next thing to try in my view – which was not tried due to time and compute cost – would be to do a train/valid/test split in the *data* (so $m_{bb\gamma\gamma}$ and m_{bb} values), then within that training set, doing some kind of k-fold validation to select hyperparameters across the different m_X, m_S points, i.e. removing random permutations of points at a time, then select the hyperparameters that cause the best average generalization to those removed points. Ensembles of flows with those hyperparameters would then be trained, and model selection performed with the valid set, then assessed on the test set. This foregoes our ability to precisely benchmark the interpolation performance as above, but any such assessment would inherently bias both model selection and apparent interpolation ability (the models may not interpolate well in other regions).

9.6 Interpolation between overall yields

In addition to the method presented in Section 9.5, there's a missing component: the overall normalization of the produced histograms. This is important from the perspective of interpretation of the signal strength μ , which represents the relative overall cross-section of $X \rightarrow SH$ multiplied by the branching ratios for $S \rightarrow bb$ and $H \rightarrow \gamma\gamma$. Why? Consider that events are generated with some assumed cross-section, and that information is encoded in the event

weights. If we do not provide this information as a normalization when inputting predicted counts from simulation into our statistical model, then the resulting signal strength limits will not accurately reflect the cross-section used, since the counts are incorrectly normalized. We then desire a second, simpler interpolation across the space of the total event count per process, which is the *sum of the event weights*.

9.6.1 Gaussian process interpolation

A flexible class of models that come with a notion of uncertainty are **Gaussian processes** (GPs). I include only a brief description; a working knowledge of GPs is not needed to gauge the quality of the results, but one can find that in the excellent article in Görtler, Kehlbeck, and Deussen (2019). To describe how we'd use GPs in this case, give each member the set of signal mass grid points (m_X, m_S values) a corresponding label for the sum of the event weights ($\sum_i w_i$) produced for that mass tuple. Each of these m_X, m_S values represents a random variable that we can model as having a normal distribution over the yields, where the means are often either zero or centered on the data, and the covariances are determined from a functional form which is called the *kernel*. The kernel is where the magic happens in GPs, and acts as the prior in a Bayesian inference context. The kernel parameters are subsequently fit to the training data.

Speaking of inference, we're then interested in inferring the values of $\sum_i w_i$ for new, unseen pairs of m_X, m_S values. By treating the joint distribution of the test and training points as a multivariate normal, with dimensions equal to the size of each set of points combined, we can condition this distribution on just the training data to get the distribution of the points in test set only. Since normal distributions are closed under conditioning, the resulting distribution will also be a multivariate normal; predictions for these points are then just samples from this distribution, which lends itself naturally to the notion of uncertainty, since we can include intervals of our choosing from that distribution along with the predicted samples.

Applying all this leads to the set of predicted values from this conditional distribution shown in Figure 9.16, where the left-hand plot shows the interpolated yield predictions, and the right-hand plot shows the corresponding relative uncertainties. The exact functional form of the kernel was chosen somewhat arbitrarily; I took many combinations of common kernels, and applied k-fold validation (with 10 folds) across the training points, then chose the form that minimized the average absolute error divided by the uncertainty from the GP (c.f. the pull from Equation 9.1). We can see that the bottom-left hand corner is white, which represents the model predicting negative yields. This is not considered problematic, as this region is outside the realm of interpolation, which is the planned context in which this would be used. Moreover, one can notice in the right-hand plot the increase in relative uncertainty as we go to the bottom-left hand corner (to nearly 100% for some values) despite that being a region of high data density. This is attributed to the fact that there is a very rapid variation in the yields in this corner of parameter space, which can be seen in the left-hand plot with the concentration of blue lines.

Functional form of the kernel of Gaussian Process (GP) fitted to all points:
 $1.24^{**2} * \text{RBF}(\text{length_scale}=185) + 0.00345^{**2} * \text{RBF}(\text{length_scale}=2.84) + \text{WhiteKernel}(\text{noise_level}=0.0459)$

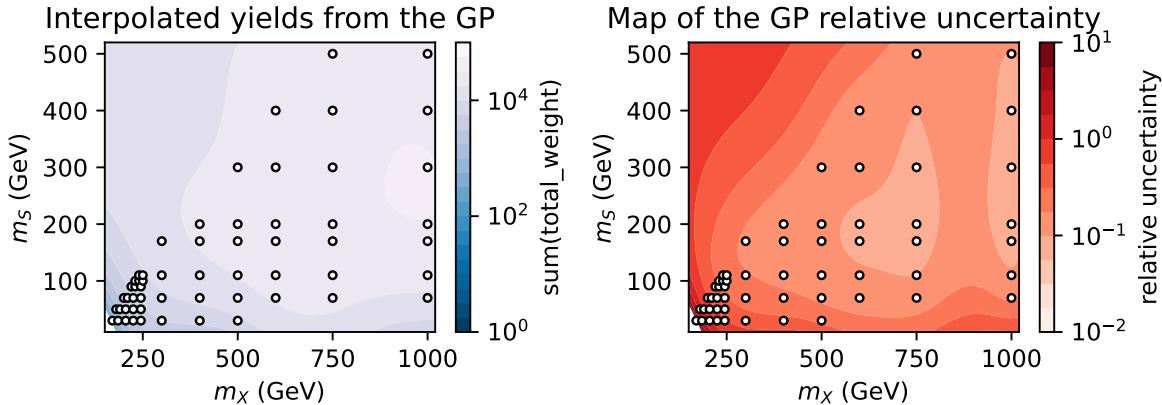


Figure 9.16: Left: Plot of the interpolated yields using a Gaussian process model, with the full post-fit kernel function described in the top of the plot. Right: The map of the corresponding uncertainties for the GP predictions.

9.7 A new flow-based observable s_{flow}

In addition to the work above, I had one more idea for this analysis. It results from thinking about the fact that we've trained a continuous likelihood function $p(m_{bb\gamma\gamma}, m_{bb}|m_X, m_S)$, but are in a sense throwing some of this information away by discretizing the result. The idea presented here tries to make use of this information from a practical standpoint, and not necessarily an optimality one.

The fit strategies proposed are both clearly effective, but they both have their shortcomings:

- The 2-D fit is *simple* and *powerful*, but suffers from the *high number of bins* needed to compute the likelihood, leading to things like ad-hoc region selection to reduce the bins we include.
- The pNN strategy is much more *efficient*, as a 1-D distribution is far more simple to compute from an inference perspective. However, we need to *assign signal masses to background*, which don't exist and so could affect our performance.

To address these points, we can be inspired by the literature for **learning likelihood ratios**, e.g. the likelihood ratio trick (Cranmer, Pavez, and Louppe 2015), where we exploit the fact that a perfect 1-D classifier between signal and background trained with binary cross-entropy would learn the distribution

$$s^*(x) = \frac{p_{\text{sig}}(x)}{p_{\text{sig}}(x) + p_{\text{bkg}}(x)} ,$$

which is then typically rearranged to construct the likelihood ratio of signal and background in terms of s^* . Here, x would be our variables of interest for classifying, e.g. $x = m_{bb\gamma\gamma}, m_{bb}$. If we were to do this using our m_X and m_S values (i.e. the pNN classifier), our signal distribution is then parametrized by m_X and m_S , so we may expect something more like

$$s^*(x|m_X, m_S) = \frac{p_{\text{sig}}(x|m_X, m_S)}{p_{\text{sig}}(x|m_X, m_S) + p_{\text{bkg}}(x)} .$$

This distribution $p_{\text{sig}}(x|m_X, m_S)$ is directly the product of our work with signal interpolation! If, then, we could learn a background distribution in the same way (e.g. with an unconditional flow), we could construct the observable

$$s_{\text{flow}}(x|m_X, m_S) = \frac{q_{\text{sig}}^{(\text{flow})}(x|m_X, m_S)}{q_{\text{sig}}^{(\text{flow})}(x|m_X, m_S) + q_{\text{bkg}}^{(\text{flow})}(x)} , \quad (9.2)$$

where the distribution $q_{\text{sig}}^{(\text{flow})}(x|m_X, m_S)$ is the output from training the flow interpolation model, and $q_{\text{bkg}}^{(\text{flow})}(x)$ comes from training a flow to learn the background distribution over x . By constructing s_{flow} , we're making something that – in the limit of well-modelled distributions for signal and background – could provide some notion of optimality when it comes to discriminating power. Moreover, unlike the pNN, we'd be explicitly modelling the background component of this, and don't have to assign values of the truth masses to the background points during training. We can also include a notion of uncertainty; if we model the flows using *ensembles* as in Section 9.5, each likelihood value will have separate predictions from each member of the ensemble, which we can average and take the standard deviation of to get uncertainties for each flow. With a bit of error propagation, we then construct the way overcomplicated formula of

$$\begin{aligned} s_{\text{flow}}(x|m_X, m_S) \pm \sigma_s &= \frac{q_{\text{sig}}^{(\text{flow})}(x|m_X, m_S) \pm \sigma_{\text{sig}}^{(\text{flow})}}{\left(q_{\text{sig}}^{(\text{flow})}(x|m_X, m_S) \pm \sigma_{\text{sig}}^{(\text{flow})}\right) + \left(q_{\text{bkg}}^{(\text{flow})}(x) \pm \sigma_{\text{bkg}}^{(\text{flow})}\right)} , \\ \Rightarrow \sigma_s &= \sqrt{\frac{\left(q_{\text{sig}}^{(\text{flow})}(x|m_X, m_S)\sigma_{\text{bkg}}^{(\text{flow})}\right)^2 + \left(q_{\text{bkg}}^{(\text{flow})}(x)\sigma_{\text{sig}}^{(\text{flow})}\right)^2}{\left(q_{\text{sig}}^{(\text{flow})}(x|m_X, m_S) + q_{\text{bkg}}^{(\text{flow})}(x)\right)^4}} . \end{aligned} \quad (9.3)$$

Only a small amount of prototyping of s_{flow} was carried out, which I'll talk about here. To model Equation 9.3, the crucial ingredient we're missing is the background flow $q_{\text{bkg}}^{(\text{flow})}(x)$; it may be desirable to split this up into explicitly modelling processes, but this was not explored, and just the overall shape was learned. Following the same prescription as Section 9.5, but without any conditioning and a train/test split on the data points themselves, I trained a flow to model the (weighted) background shape. A comparison between the learned flow distribution and the data histogram can be found in Figure 9.17.

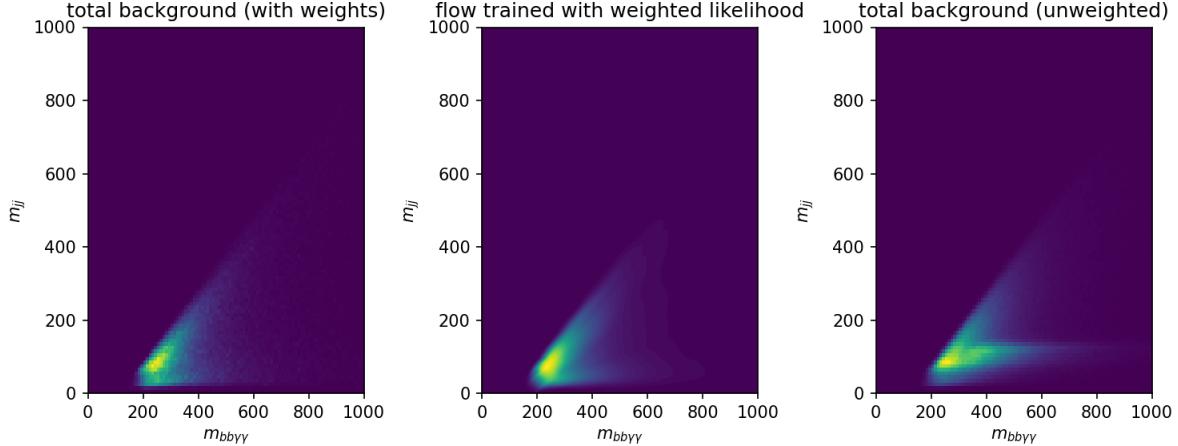


Figure 9.17: Left: Background histogram including event weights. Middle: Learned flow distribution. Right: Background histogram without event weights.

Satisfied that the shape is good, we move swiftly on to view some of the example distributions given by Equation 9.3 using this flow and one of the results from the many training configuration tried in Section 9.5. We find these distributions in Figure 9.18, where we plot the value of s_{flow} for an equal number of points from both background and signal distributions (244637 – the length of the background test set), using their values of $m_{bb\gamma\gamma}, m_{bb}$ as input. Note that the points shown are all unseen points from the perspective of the signal flow, and the background data is also from the test set partition from the training, so none of the data has been seen by either flow. Despite this, the observable shows some great promise for discriminating between signal and background, with the distributions being largely separated. The cases that perform slightly worse are those where the background Monte Carlo distribution peaks, e.g. the point $m_X = 300$ GeV, $m_S = 170$ GeV, but even then the performance is still highly discriminatory.

9.8 Future and outlook

There are many ideas here – I’m unsure how many will make it into the final analysis product, but the interpolation has gotten more mature since I wrote this section, though it still suffers from some of the drawbacks listed. In particular though, it now trains on *all* the mass points, and will be assessed with some newly generated events from previously non-existent mass points that definitely fall in the interpolation range.

Those that are ATLAS-inclined are invited to look at the internal note we just published, which includes much more detail on the overall analysis: ANA-HDBS-2021-17-INT1.

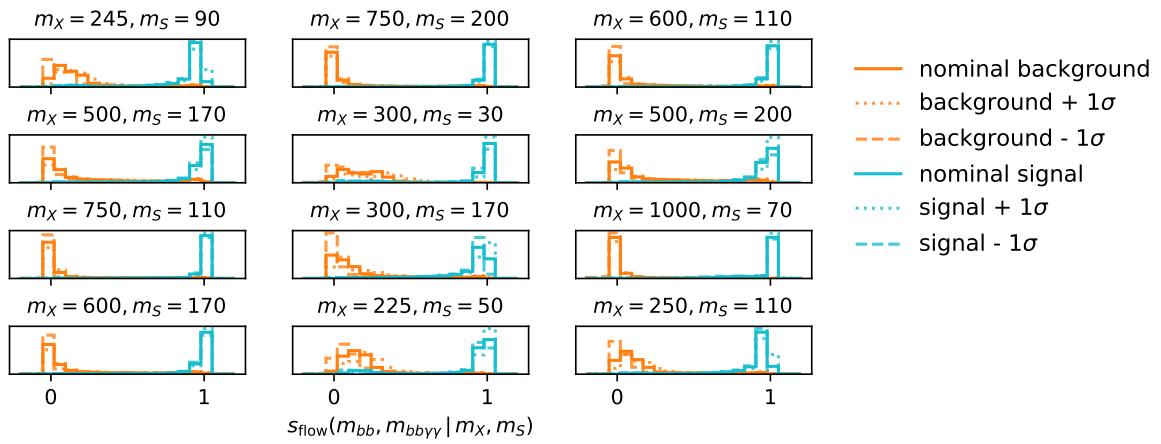


Figure 9.18: Plots of the distribution of s_{flow} for a variety of test set signal points, where an even number of points are provided of either signal or background.

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A Results when optimizing a neural network observable and binning simultaneously

A.1 5-bin observable

Metrics

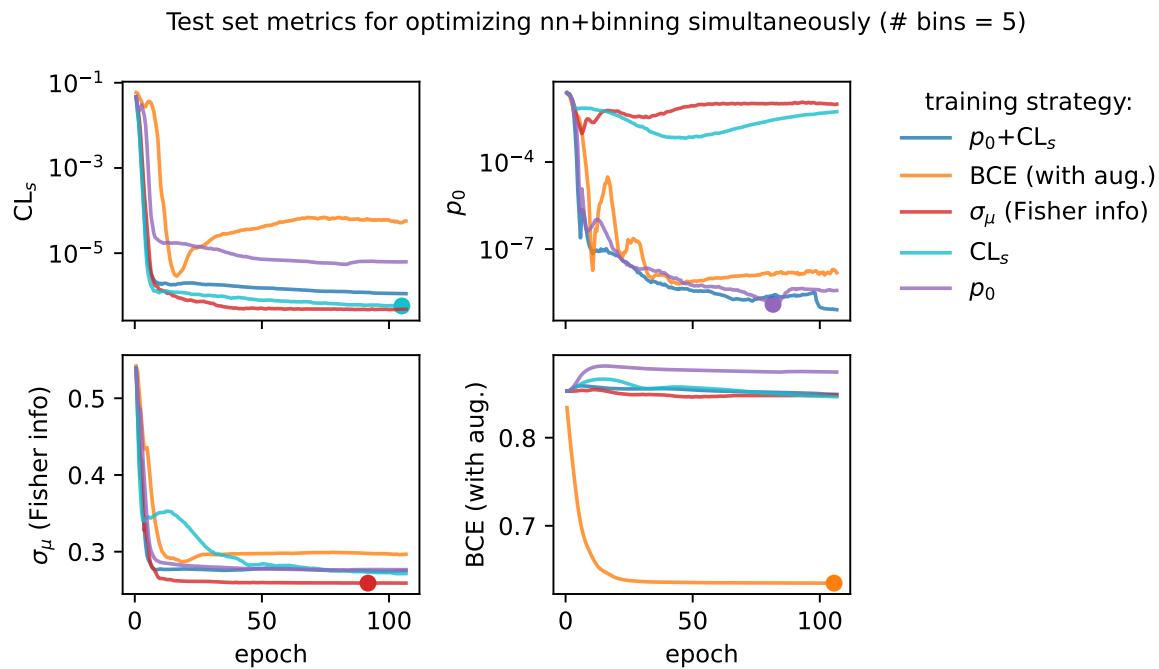


Figure A.1: Plots of the different metrics calculated on the test set for different training strategies using a 5-bin neural network observable. The results are averaged across 9 random seeds for the weight initializations. The scatter points on some of the curves represent the model that we would select in practice if using that training strategy (provided we decide to use the loss as the selection metric).

Example models learned when optimizing p_0 (# bins = 5)

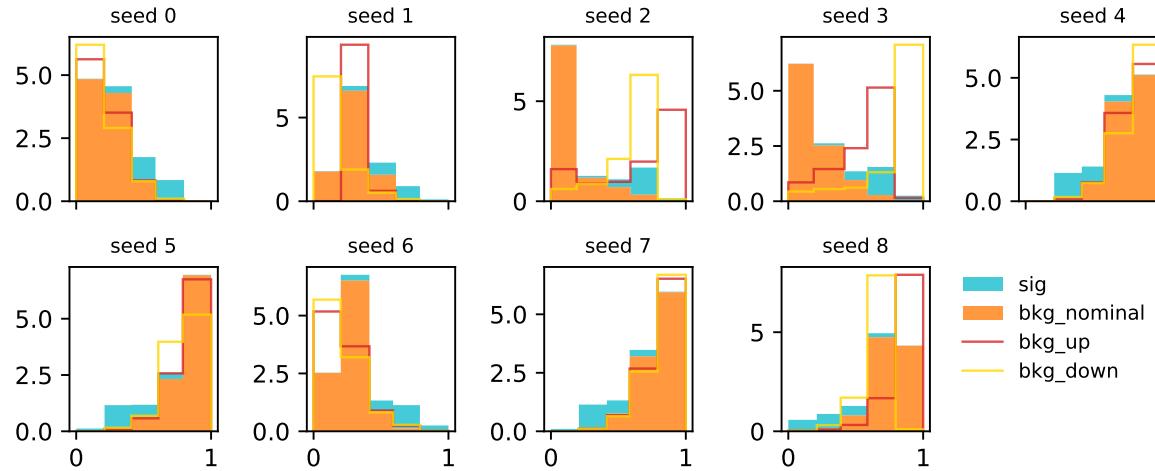


Figure A.2: Histograms from optimizing with respect to the discovery p -value p_0 .

Example models learned when optimizing CL_s (# bins = 5)

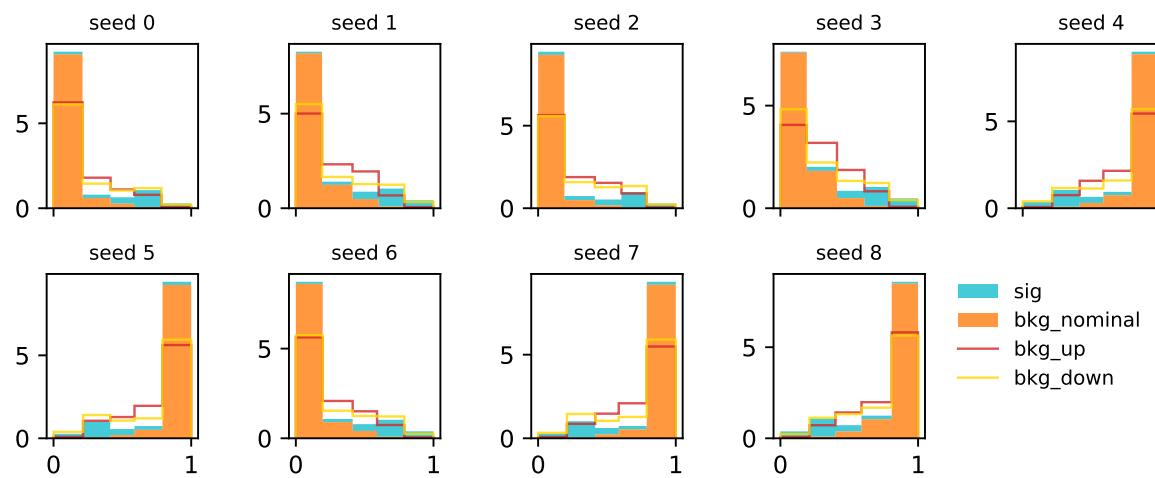


Figure A.3: Histograms from optimizing with respect to the CL_s .

Example models learned when optimizing $p_0 + \text{CL}_s$ (# bins = 5)

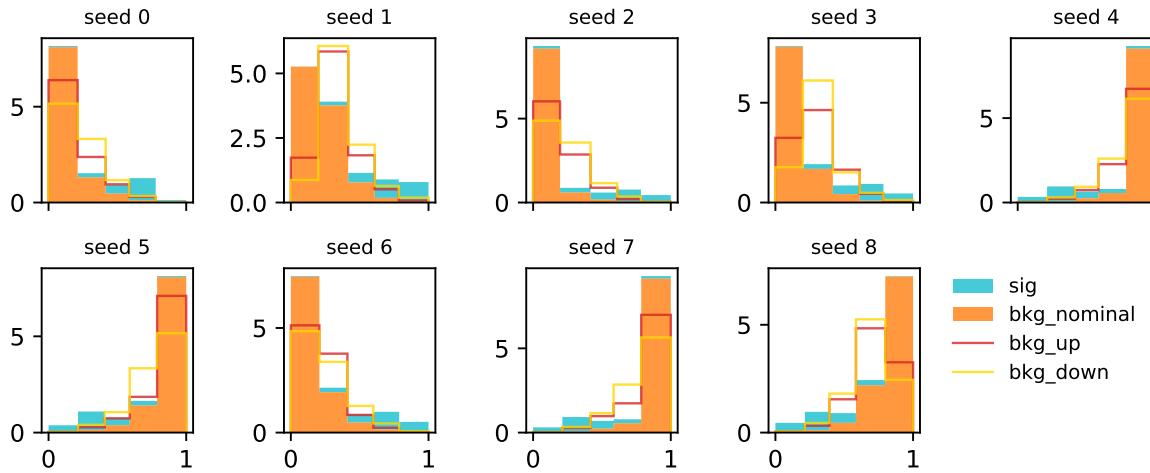
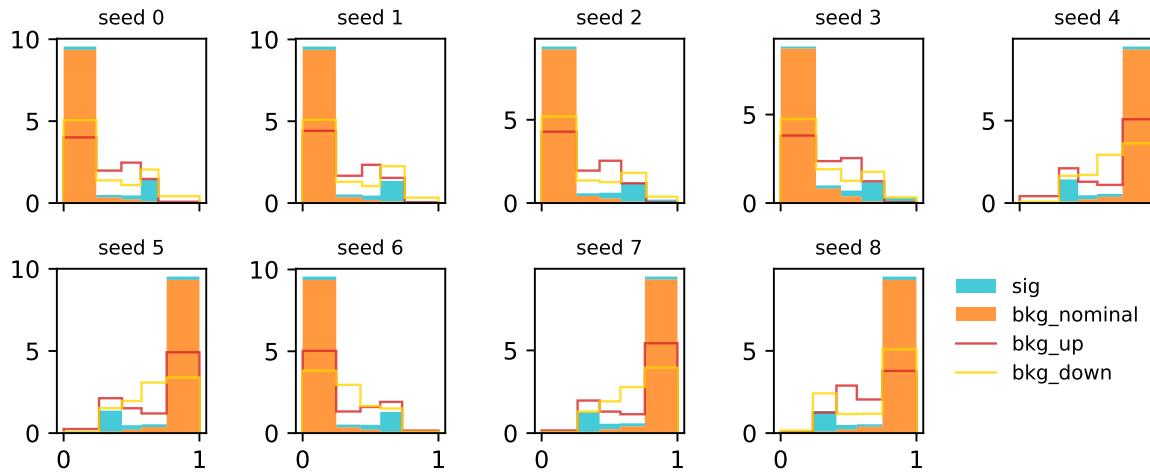


Figure A.4: Histograms from optimizing with respect to a combination of discovery p -value and CL_s .

Histograms

Example models learned when optimizing σ_μ (Fisher info) (# bins = 5)



Example neural network boundaries learned when optimizing p_0 (# bins = 5)

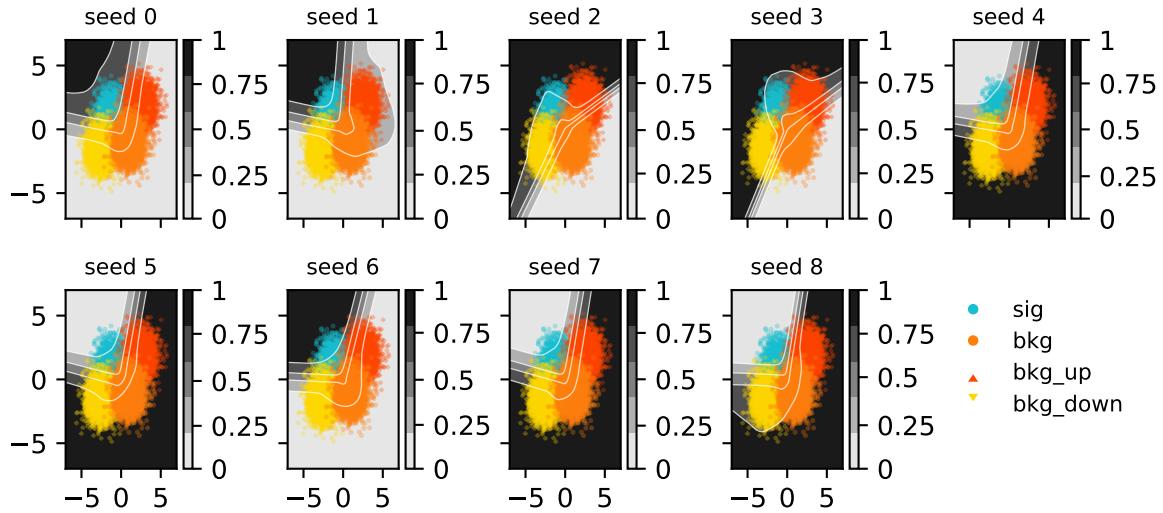


Figure A.5: Histograms from optimizing with respect to the discovery p -value p_0 .

Example neural network boundaries learned when optimizing CL_s (# bins = 5)

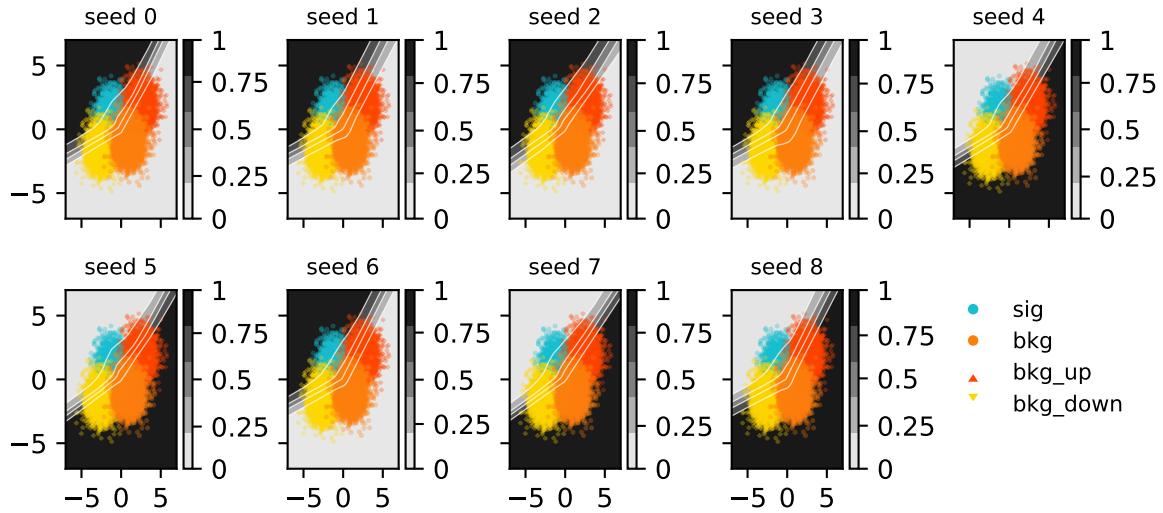


Figure A.6: Histograms from optimizing with respect to the CL_s .

Example neural network boundaries learned when optimizing $p_0 + \text{CL}_s$ (# bins = 5)

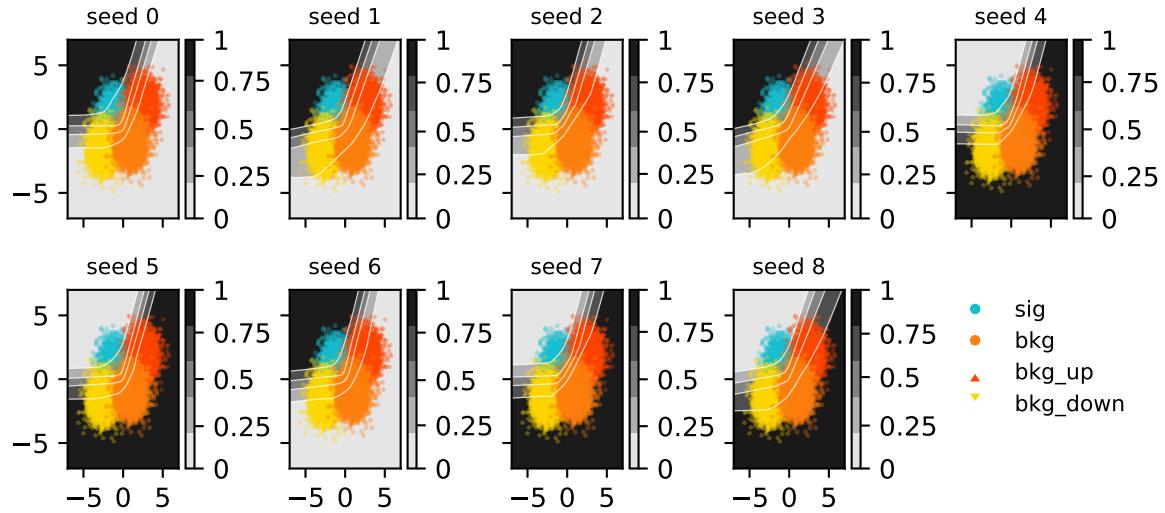


Figure A.7: Histograms from optimizing with respect to a combination of discovery p -value and CL_s .

Example neural network boundaries learned when optimizing σ_{μ} (Fisher info) (# bins = 5)

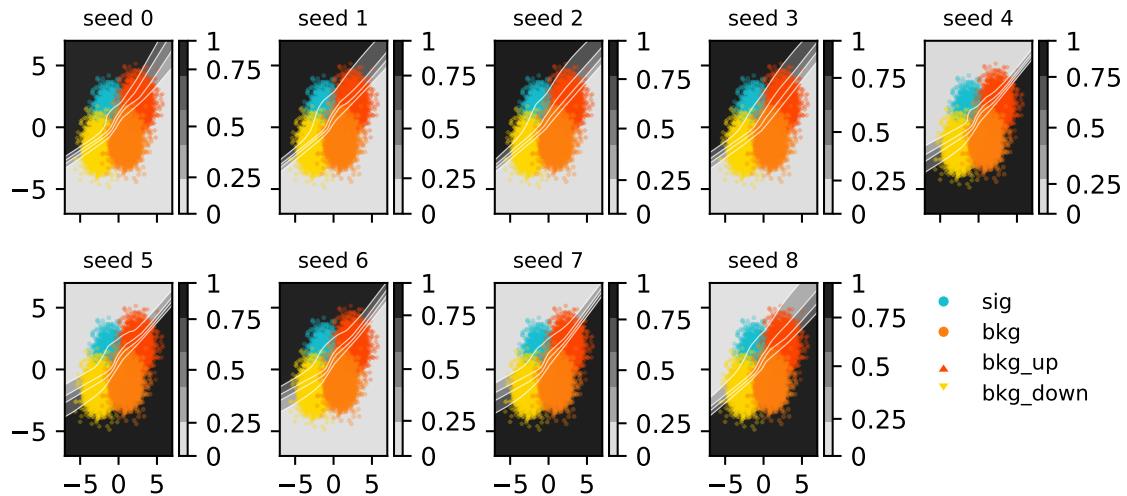


Figure A.8: Histograms from optimizing with respect to the Fisher information estimate of $\sigma_{\hat{\mu}}$.

Neural network contours in data space

A.2 20-bin observable

Metrics

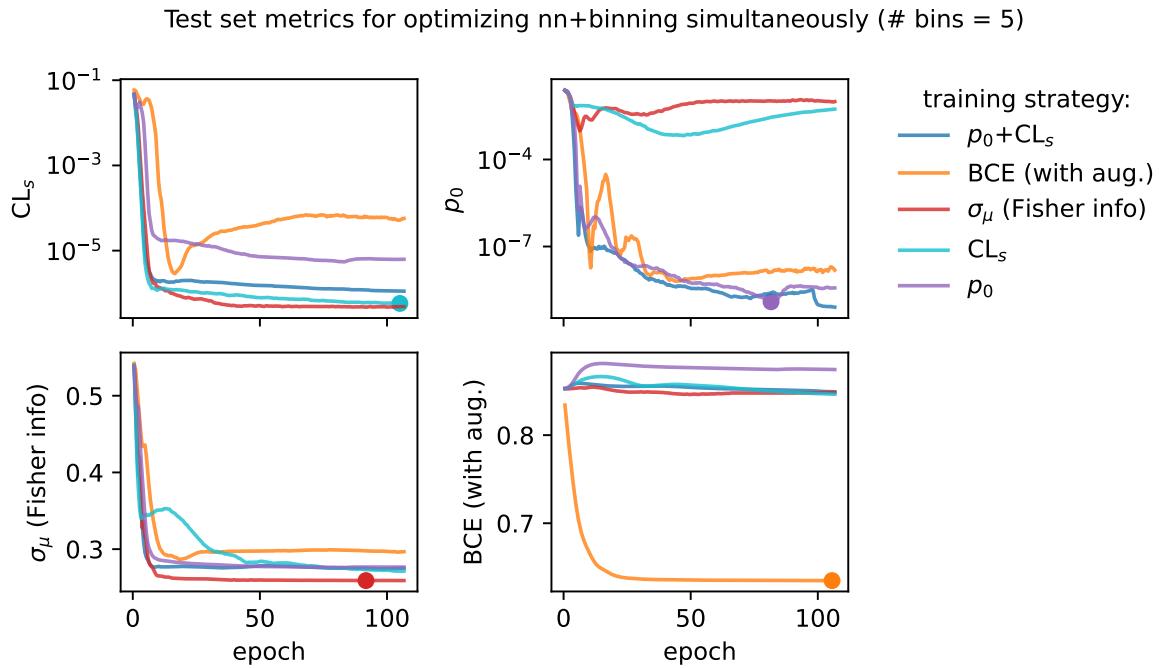


Figure A.9: Plots of the different metrics calculated on the test set for different training strategies using a 20-bin neural network observable. The results are averaged across 9 random seeds for the weight initializations. The scatter points on some of the curves represent the model that we would select in practice if using that training strategy (provided we decide to use the loss as the selection metric).

Histograms

Neural network contours in data space

Example models learned when optimizing p_0 (# bins = 20)

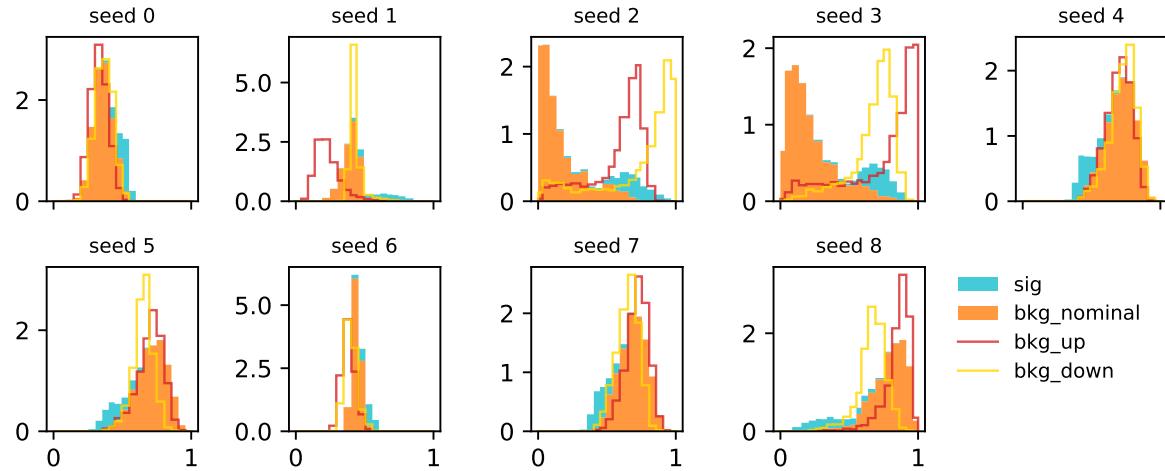


Figure A.10: Histograms from optimizing with respect to the discovery p -value p_0 .

Example models learned when optimizing CL_s (# bins = 20)

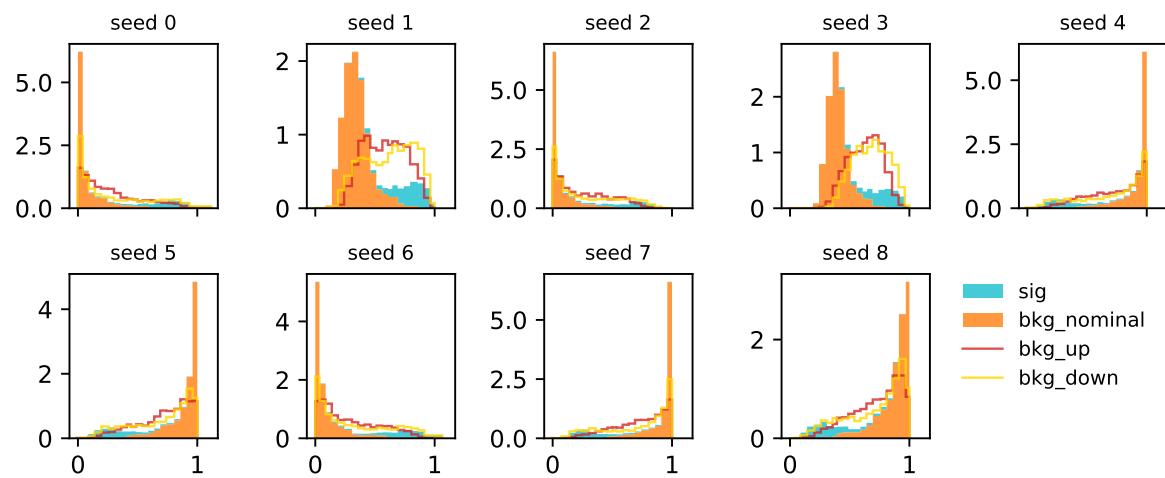


Figure A.11: Histograms from optimizing with respect to the CL_s .

Example models learned when optimizing $p_0 + \text{CL}_s$ (# bins = 20)

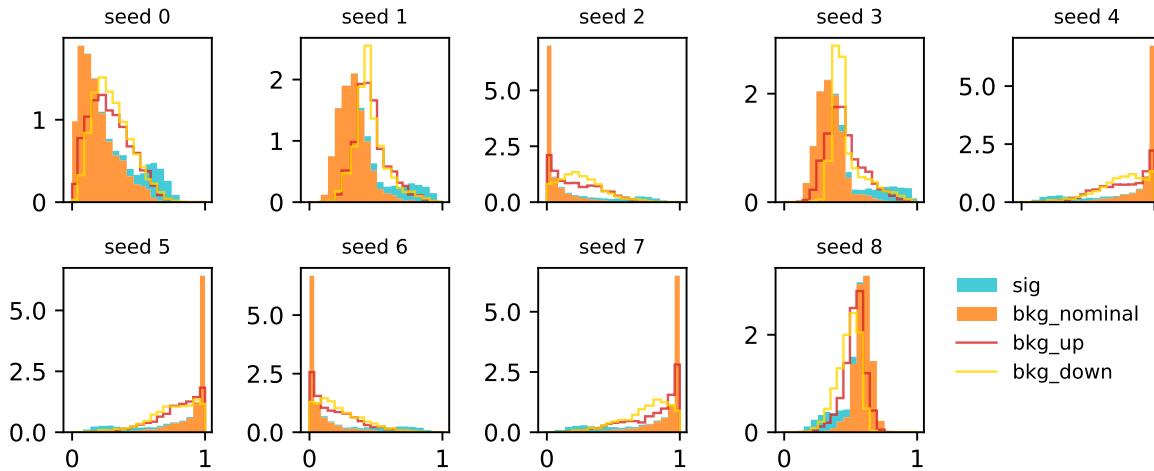


Figure A.12: Histograms from optimizing with respect to a combination of discovery p -value and CL_s .

Example models learned when optimizing σ_{μ} (Fisher info) (# bins = 20)

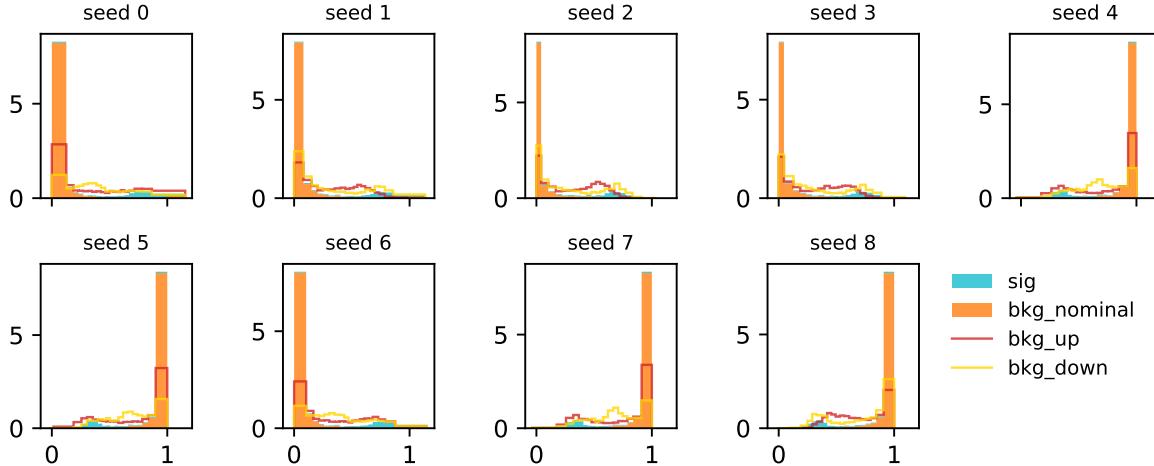


Figure A.13: Histograms from optimizing with respect to the Fisher information estimate of $\sigma_{\hat{\mu}}$.

Example neural network boundaries learned when optimizing p_0 (# bins = 20)

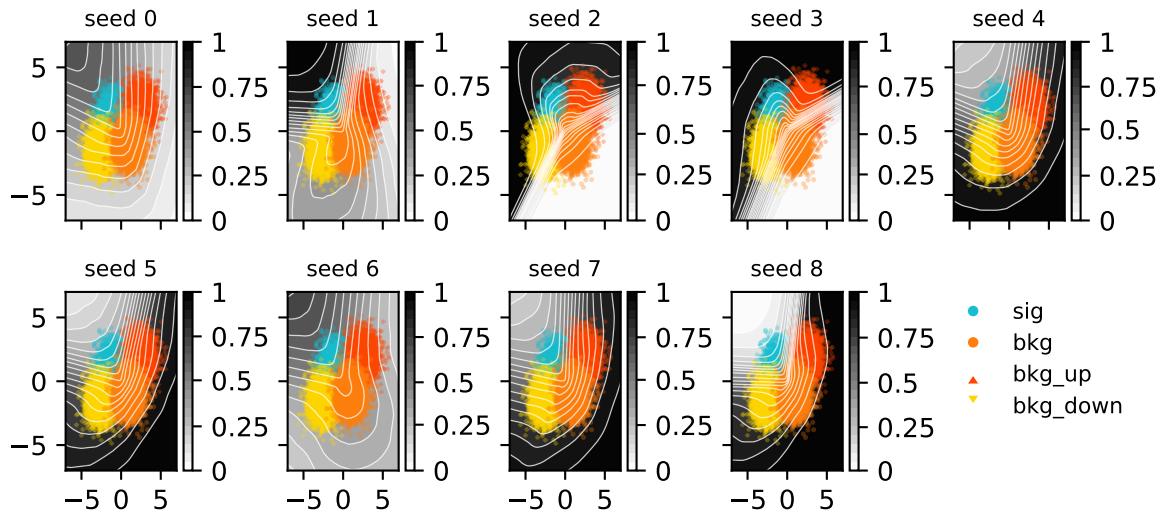


Figure A.14: Histograms from optimizing with respect to the discovery p -value p_0 .

Example neural network boundaries learned when optimizing CL_s (# bins = 20)

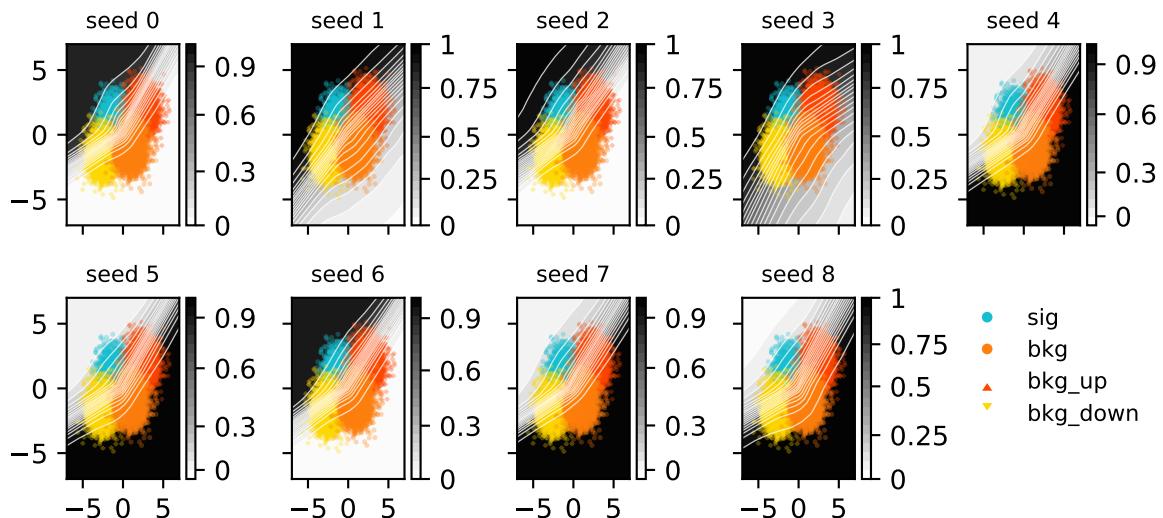


Figure A.15: Histograms from optimizing with respect to the CL_s .

Example neural network boundaries learned when optimizing $p_0 + \text{CL}_s$ (# bins = 20)

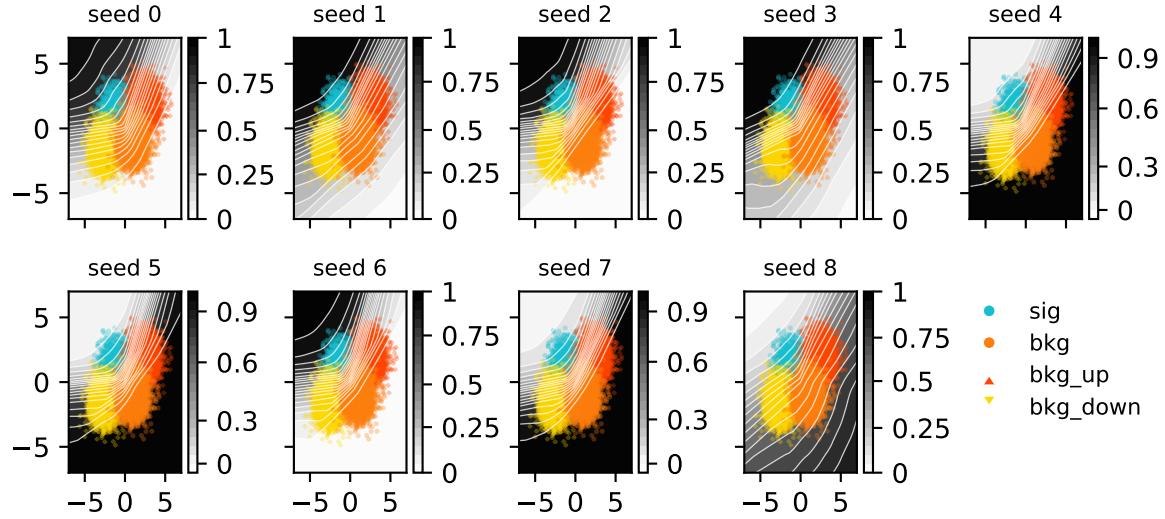


Figure A.16: Histograms from optimizing with respect to a combination of discovery p -value and CL_s .

Example neural network boundaries learned when optimizing σ_μ (Fisher info) (# bins = 20)

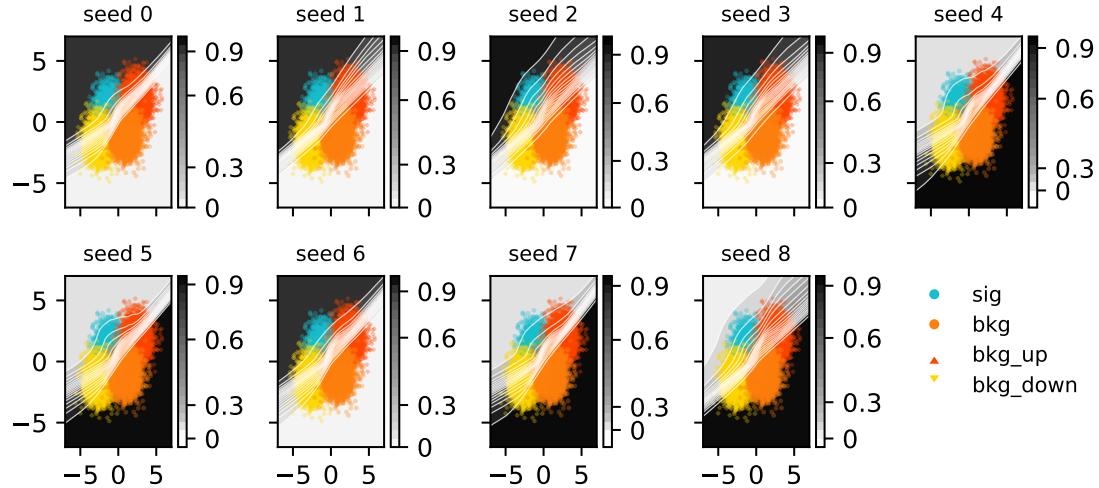


Figure A.17: Histograms from optimizing with respect to the Fisher information estimate of σ_μ .