Threshold optimization and Bayesian inference on the XENON1T experiment

by

Arjen Wildeboer
10269045

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Supervisor/Examiner: dhr. prof. dr. M.P. Decowski
Examiner: dhr. dr. M. Vreeswijk

Daily supervisor: dhr. J. Aalbers, MSc.

National Institute for Subatomic Physics
Abstract

The XENON collaboration operates the highly sensitive dark matter detector XENON1T at Gran Sasso, Italy. This thesis reports on the optimization of the thresholds inside XENON1T’s data processor Pax, and examines Bayesian inference as an alternative statistical method to set upper limits on the WIMP-nucleon cross section.

The hitfinder module inside Pax determines whether there are hits inside a PMT pulse. A hit is detected if the pulse passes a certain threshold. The optimal upper threshold and lower threshold are determined, such that the hitfinder is able to fully integrate the hits and to find as many photoelectron signals in XENON1T’s first science run data as possible, while it triggers as few as possible when there are no photons.

The statistical method Bayesian inference is applied to set an upper limit on the WIMP-nucleon cross section using the first science run data. A Bayesian upper limit is obtained that improves upon XENON1T’s published frequentist limit, for all WIMP masses. Nevertheless, the sensitive dependence of the upper limit on the non-objective choice for a specific prior makes Bayesian inference an unsuitable method for setting the upper limit for the XENON1T experiment.
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Chapter 1

Introduction

One of the most intriguing open challenges in physics is detecting the particle that is responsible for dark matter. Astrophysical observations have established that approximately 85% of the mass of the universe consists of this dark matter. Despite its overwhelming abundance, the dark matter particle has never been directly observed. It is believed that the particle only interacts weakly with ordinary matter, which makes it a difficult target for detection. To date, no dark matter experiment has been able to prove that the particle exists. Instead, they have reported upper limits on the dark matter interaction cross section.

One of these detectors is the XENON1T detector, which is designed and operated by the XENON collaboration. This detector currently holds the record for achieving the lowest background in a dark matter detector. It is located 1400 meter underground in Gran Sasso, Italy. The goal of this detector is to explore new parameter space, and either detect a dark matter particle or set a stricter upper limit on the cross section.

This thesis is the result of one year’s research at the Nikhef XENON group. The first goal of this work is to optimize the thresholds of the hitfinder module. The hitfinder module is the subsystem of XENON1T’s data processor Pax that determines whether there are hits inside a pulse of a PMT. The second goal is to use Bayesian inference as an alternative statistical method to set upper limits on the dark matter cross section, using the first science run data of XENON1T.

The content is structured as follows. First, Chapter 2 gives an introduction to dark matter theory. Thereafter, Chapter 3 focuses on the detection principle of the XENON1T detector. Next, Chapter 4 discusses the data processor Pax and its subsystems, among which the hitfinder module. Following, Chapter 5 and 6 respectively discuss the optimization of the upper threshold and the lower threshold of the hitfinder module. Continuing, Chapter 7 discusses the concept of Bayesian inference as a statistical framework to set an upper limit on the cross section. Finally, Bayesian inference is applied in Chapter 8, where a Bayesian upper limit on the cross section is set using the first science run data.
CHAPTER 1. INTRODUCTION
Chapter 2

Dark Matter

Only a small portion of the objects in our Universe, such as stars, planets and gas clouds, consists of ordinary matter. Ordinary matter is all the matter composed of particles from the Standard Model of particle physics. The largest part of the energy density in our Universe is accounted by two other contributors, which are called dark matter and dark energy. The names refer to their extremely weak interaction with photons. They fill up the additional mass component and energy component that is missing in the Universe.

The precise particle that accounts for the missing mass remains unknown until today. Nevertheless, it is known that the dark matter (DM) is responsible for holding our Milky Way together and that it influences the large-scale structure of the Universe.

Precise measurements of the temperature of the Cosmic Microwave Background (CMB) performed by the Planck Collaboration show that approximately 70% of the energy content of our Universe comes from dark energy. The second largest contribution of 25% is dark matter, while the ordinary baryonic matter only accounts for less than 5% of the total energy content [1]. This matter-energy breakdown of our Universe is shown in Figure 2.1.

Figure 2.1: Breakdown of the matter-energy components of the Universe.
The cosmological model that effectively elucidates the matter-energy fractions in the cosmos is the $\Lambda$-Cold Dark Matter ($\Lambda$CDM) model. It is a model that accurately characterizes the evolution of the Universe. The name refers to the cosmological constant $\Lambda$, which is associated with the dark energy density. Cold Dark Matter refers to the dark matter density. The dark matter in the model is described as being cold, which means that its velocity is non-relativistic.

The relative abundance of baryons, dark matter and dark energy as a fraction of the critical energy density has been exactly calculated using the CMB [1]:

\[
\begin{align*}
\text{Dark Energy } \Omega_{\Lambda} &= 0.685 \pm 0.013 \quad (2.1) \\
\text{Cold Dark Matter } \Omega_{c}h^{2} &= 0.1198 \pm 0.0015 \quad \Rightarrow \quad \Omega_{c} = 0.2647 \pm 0.0033 \quad (2.2) \\
\text{Baryons } \Omega_{b}h^{2} &= 0.0225 \pm 0.00016 \quad \Rightarrow \quad \Omega_{b} = 0.04917 \pm 0.00035 \quad (2.3)
\end{align*}
\]

where $\Omega_{i} = \rho_{i}/\rho_{c}$, $\rho_{i}$ is the actual observed density, $\rho_{c}$ is the critical density of the Universe, and $\Omega_{b}$ and $\Omega_{c}$ are derived using the reduced Hubble constant $h = H_{0}/(100 \text{ km s}^{-1} \text{ Mpc}^{-1}) \approx 0.6727$.

The critical energy density is the energy density at which the Universe has a flat geometry. The assumption that the Universe has a flat geometry results in the constraint that the total density $\Omega_{\text{tot}}$ is equal to 1. The BOOMERanG experiment discovered that the total density is indeed equal to 1 with only a 0.4% error margin [2]. A flat universe is also assumed in the $\Lambda$CDM model:

\[
\sum_{i} \frac{\rho_{i}}{\rho_{c}} = \sum_{i} \Omega_{i} = \Omega_{\text{tot}} = 1.
\]

The abundance of dark matter throughout the Universe has been recognized for almost more than a century, yet a lot of questions remain unanswered. Especially on a microscopic level much is unknown. For example, whether dark matter is composed of particles, and if so, how these particles interact with the known particles in the standard model. The dark matter particle has not been detected until today. Nevertheless, the first evidence that claims the existence of dark matter has already been presented almost a century ago.

This chapter introduces the most convincingly pieces of evidence for the existence of dark matter, such as the rotation curves of galaxies, the Cosmic Microwave Background, and the gravitational lens. The various particle candidates for dark matter are presented as well and in particular the most popular candidate: the Weakly Interacting Massive Particle (WIMP). Thereafter the different detection principles and corresponding limits are expounded.
2.1 Evidence for dark matter

Since dark matter is neither emitting nor absorbing light, all modern telescopes that detect photons are not able to directly detect the matter. It is however possible to indirectly observe dark matter due to its interaction with gravity. For example, by studying the movement of visible objects such as stars and interstellar clouds, it can be shown that there should be more mass in our Universe than directly observed. The most compelling evidence for the existence of dark matter comes from the rotation curves of galaxies, the Cosmic Microwave Background, and the gravitational lens.

2.1.1 Rotation curves

The rotation curve of a galaxy shows the measured orbital velocity of the objects in the galaxy as a function of their distance from the corresponding galactic center. It was in 1933 when Fritz Zwicky studied the rotation curve of the Coma Cluster. By observing the movements in the cluster, he estimated the amount of mass that the cluster contained. He tried to measure the same mass again using the amount of light that was emitted from the cluster. Because the amount of mass implied by the movements was much higher than the amount of mass measured using the visible matter, Zwicky concluded that there must be more mass in the Coma Cluster than previously thought [3]. This mass he called dark matter.

It took another fifty years before the theory of dark matter became generally accepted. In 1978, Vera Rubin observed that 21 spiral galaxies had a different velocity than what is expected from Newtonian dynamics [4]. She used the assumption that stars in the disk of a spiral galaxy move in the same way as planets in our solar system. The expected rotation curve for a given mass distribution is then found by setting the gravitational force equal to the centripetal force:

\[ \vec{F}_C = \vec{F}_G \implies \frac{m v^2}{r} = \frac{G M(r) m}{r^2} \implies v(r) = \sqrt{\frac{G M(r)}{r}}. \tag{2.5} \]

If it is furthermore assumed that the mass \( M \) is concentrated in the center, such that it no longer depends on the distance from the galaxy center \( r \), it follows from Equation 2.5 that the average orbital velocity of the objects in the galaxy is expected to behave as \( v(r) \propto \frac{1}{\sqrt{r}} \).

However, observations of the rotation curve of spiral galaxies show that the stars in these galaxies do not have velocities in line with this relation. Figure 2.2 shows the measured rotation curve of the spiral galaxy NGC 6503 [5]. It displays the circular velocity of stars as a function of the distance from the galactic center. The velocities do not show the \( \propto \frac{1}{\sqrt{r}} \) relationship that was derived in Equation 2.5.
At large radii outside of the central bulge, the orbital velocities of the stars (solid line) do not go to zero as expected, and instead stay approximately constant.

The contributions from the luminous mass of the bulge disk (dashed line) and the interstellar gas (dots) do not add up to the mass content of the observed flat velocity distribution. A dark matter halo component (dash-dot line) needs to be added in the galaxy to explain the observed rotation curve [5].

The discrepancies between the observations and the predictions from Newton’s law thus imply the existence of a dark matter component in the halo of galaxies that extends far beyond the range of the stars and gas in the galaxy. The existence of this dark halo component has also been predicted by the Cosmic Microwave Background and the gravitational lensing effect.

Figure 2.2: Rotation curve of the galaxy NGC 6503 showing the disk and gas contribution plus the additional dark matter halo contribution needed to match the data [5].
2.1. EVIDENCE FOR DARK MATTER

2.1.2 Cosmic microwave background

According to the Big Bang theory, the early Universe consisted of a plasma containing all elementary particles that continuously interacted with each other. At that time, approximately 100,000 years after the big bang, the Universe was filled with a hot ionized gas, which had some slight deviations in density. While the Universe expanded and the temperature dropped, previously uncoupled protons and electrons began to form neutral atoms. This happened during the epoch of recombination. Atoms could no longer absorb photons, resulting in free photons traveling through the Universe without interaction with matter. These photons are observed today as the Cosmic Microwave Background radiation. The Cosmic Microwave Background (CMB) is thus the thermal radiation leftover from the time of recombination in Big Bang cosmology. The small changes in the intensity of the CMB across the sky give a map of the slight deviations in the density of the plasma in the early Universe. Such a map has been made with various telescopes. Figure 2.3 shows the CMB made by the space-based Planck telescope [6].

![Figure 2.3: Map of the Cosmic Microwave Background.](image)

Quantum fluctuations in the early Universe cause the fluctuations in the radiation. They started the matter accumulation resulting in today’s galaxies.

Research on the CMB has revolutionized the study of cosmology. Any proposed cosmological model of the Universe, such as the ΛCDM model, should explain the radiation in the CMB. Even though the radiation seems almost uniform in all directions, small temperature deviations show a specific pattern. These deviations vary with the size of the region examined. They are similar to what is expected from thermal variations, caused by tiny quantum fluctuations of matter in a small space, that expanded to the size of the Universe. Therefore it is thought that the tiny fluctuations at the beginning of the Universe have grown over time due the gravity, and eventually started the formation of galaxies and galaxy clusters.
The mean temperature fluctuations at various distances expressed as a solid angle in the Universe can be found using data from the Planck telescope \[\text{(7)}\]. Figure 2.4 shows this spectrum as a function of the angular scale. The horizontal axis displays the multipole moment $\ell$, which is defined as the difference between two directions in terms of their angular separation $\Theta$: $\ell = 180^\circ / \Theta$. Larger scales in the sky coincide with lower values for $\ell$. The vertical axis shows for each value $\ell$ the amount of variation in the temperature of the CMB.

One large peak is followed by smaller peaks at smaller angular differences (or higher multipole moments). With the use of the laws of General Relativity and a series of spherical harmonics, it is possible to fit the six free parameters from the $\Lambda$CDM model (green line) very accurately to the power spectrum data (red dots). Using the relative heights of the peaks, it can be deduced that the data is consistent with a flat Universe dominated by a vacuum energy density. The baryon density, the dark matter density, the dark energy density and the cosmological constant can be found with this fitted $\Lambda$CDM model, resulting in the abundances given in Equations 2.1, 2.2 and 2.3. The angular power spectrum shows that the $\Lambda$CDM model, which assumes a cold dark matter component, is consistent with the observations on the CMB.

![Figure 2.4: The CMB power spectrum as a function of angular scale \[\text{(7)}\]. The green line is the best-fitting $\Lambda$CDM model to the red data points. Constraints on various cosmological parameters are obtained from the fitted power spectrum, such as the abundance of dark matter in the Universe.](image-url)
2.1.3 Gravitational lensing

The existence of dark matter is also predicted by gravitational lenses. A gravitational lens is a relatively strong gravitational field, such as a galaxy or a black hole, that bends the light from an object behind that field. This effect can be seen when the observer, the gravitational field, and the object are positioned in a straight line. The strength of the gravitational lens depends on the position of the observer, the lens, the source and the mass distribution inside the lens.

In strong lensing, a relatively heavy object, such as a galaxy or a cluster, acts as the lens. This results in an increase of the number of images of the stellar object around the lens. Weak lensing, on the other hand, only slightly bends the path of the light, resulting in a blurred image of the stellar object that is positioned behind the lens. The amount of light that can be seen from the luminous object is then increased due to the weak gravitational lensing effect.

The strength of the deflection depends on the mass of the gravitational lens. Because of this relation, it is possible to determine the amount of mass in a star cluster with the help of the gravitational lens. Researchers have used this method to prove the presence of dark matter in the Bullet Cluster [8].

The Bullet Cluster consists of two galaxy clusters that collided approximately 150 million years ago. Without the existence of dark matter, the clusters would mostly contain a hot diffusive gas combined with a small fraction of stellar components. When such clusters collide, it is expected that the stellar objects just pass each other without collision, while the diffuse gas is slowed down due to the frictional interactions between the gas components. One would also expect that the gravitational potential lies at the center of the mass, exactly where all the merged and slowed down gas is concentrated since there is a lot more mass in the gas than in the stellar objects.

However, observations on the Bullet Cluster, shown in Figure 2.5, indicate that most mass is still separately located at the center of each cluster. This rejects the assumption that the hot gas accounts for most of the mass. The displayed mass distribution can be explained by adding a dark matter component. If the two clusters contained dark matter, which also interacts through gravity, the two centers of mass would pass through each other unaffected, precisely in line with the observations [8]. This results in strong evidence in favor of the presence of dark matter in our Universe.

Figure 2.5: The left panel shows the merging clusters. The contours of the spatial mass distribution (green lines) are measured with gravitational lensing. The right panel shows the gas clouds, which are clearly displaced from the actual centers of mass. [8]
2.2 Dark matter candidates

The existence of dark matter has been predicted by these various experiments over the past decades. The question that remains unanswered is what kind of particle dark matter is. Many theoretical models have been created describing the nature of dark matter, with each of these models taking into account the several restrictions that arise from the astrophysical observations and the various dark matter experiments.

A brief overview can be made describing the main properties that each candidate needs to satisfy. First of all, the particle needs to be abundant and massive enough to match the observations of the CMB from the previous section. Furthermore, it has to be (nearly) electromagnetically neutral, otherwise it would have been observed with regular telescopes. The studies on the CMB have also set a limit on the abundance of baryonic matter in the Universe, implying that the dark matter particle has to be non-baryonic. It should interact only weakly with the ordinary baryons in the Universe since observations of interactions with baryons have not been observed [9]. The strength of the self-interaction of dark matter should also be small, as the centers of mass in the Bullet Cluster passed almost unaffected through each other [10]. It should be non-relativistic to allow the formations of galaxies, galaxy clusters and other structures in the Universe. Furthermore, the particle has to be stable in order to play a role on cosmological time scales, from the creation of the CMB to the motions of galaxies and galaxy clusters nowadays.

None of the standard model particles meet these requirements. Therefore, a new particle has to be found that fulfills the imposed constraints. Various hypothetical particles have been proposed to explain the nature of dark matter, of which the the Weakly Interactive Massive Particle is the most popular candidate.

2.2.1 Weakly Interacting Massive Particle

A second and more widely supported paradigm for explaining the dark matter in the Universe is the Weakly Interactive Massive Particle (WIMP). This hypothetical elementary particle $\chi$ interacts only through gravity, the weak nuclear force, and possibly other interactions as long as their corresponding cross sections are smaller than the weak scale. The WIMP has a mass in the $1 \text{ GeV} - 1 \text{ TeV}$ scale, which is much larger than the standard model particles. To create such a large mass particle in an accelerator experiment requires a large amount of energy, which explains why experiment did not yet succeed in creating a WIMP.

The theory of WIMPs assumes that the particles were created in the early dense universe when there was enough energy available to create them. Due to the high temperatures, the WIMPs were in thermal equilibrium with all the other particles. While the universe expanded and cooled down, there was a point where the temperature became below the WIMP rest mass ($m_\chi$). This caused their number density to drop since the creation of WIMPs occurred less often than that they annihilated with each other into standard model particles.
2.3. DARK MATTER SEARCHES

In this WIMP-scenario, the freeze-out temperature \( T_f \) turns out to be much lower than the mass of the WIMP, which results in a WIMP number density dropping proportionally with the Boltzmann-suppression factor: \( n_\chi \propto e^{-m_\chi/T_f} \) \[1\]. If the expansion of the universe would have been slower, the particles could have stayed in a thermal equilibrium resulting in a small number of WIMPs. However, due to the faster expansion of the universe and the decreasing number of WIMPs, the probability that the WIMPs annihilated with each other became negligible. This caused a WIMP freeze-out, resulting in the dark matter density that is observed today.

An estimate for the current cosmological abundance of the WIMPs \((\Omega_\chi)\) is given in terms of its self-annihilation cross section \(\langle \sigma v \rangle\) \[12\]:

\[
\Omega_\chi h^2 = \frac{m_\chi n_\chi}{\rho_c} \simeq \frac{3 \times 10^{-27} \text{cm}^3\text{s}^{-1}}{\langle \sigma v \rangle},
\]

where \( h \) is the Hubble constant in units of 100 km s\(^{-1}\) Mpc\(^{-1}\), and \( \rho_c \) the same critical density of the Universe from Equation 2.4. To let Equation 2.6 correspond to the amount of dark matter that is observed in the universe today, a self-annihilation cross section of \(\langle \sigma v \rangle \simeq 2.2 \times 10^{-26} \text{ cm}^3\) is needed \[13\]. This value is approximately equal to what is expected for a new particle that interacts via the electroweak force in the 100 GeV mass range. This apparent coincidence is referred to as the WIMP miracle and has been the driving force behind the vast effort to detect WIMPs.

Each dark matter candidate thus has to be a stable, neutral and massive particle that does not have electromagnetic interaction with other particles. When it is also assumed that it has a weak scale interaction and a mass in the GeV-TeV range, as predicted by the WIMP miracle, it should be possible for experiments to detect dark matter directly through its weak interaction with baryons.

2.3 Dark matter searches

The WIMP miracle gives rise to the existence of dark matter at the weak scale. If there is indeed such an interaction between the WIMPs and standard model particles, there are three possible strategies to detect the dark matter. There could be the annihilation, the scattering and the production of dark matter with standard model matter, as shown in Figure 2.6. Scattering is referred to as direct detection, while the annihilation process is mentioned as indirect detection.

![Figure 2.6: Detection methods and possible interactions for dark matter (DM) and standard model particles (SM) \[14\].](image-url)
2.3.1 Production at colliders

In theory, it should be possible to produce dark matter in a particle accelerator such as the Large Hadron Collider (LHC). This can only happen if the center-of-mass energy is large enough combined with a dark matter particle that has a low mass. After creation of the dark matter, the particle itself would escape through the detectors unnoticed, however this would result in missing energy and missing momentum. The presence of dark matter can then be verified by calculating the amount of missing energy and momentum after the collision. So far dark matter has not been detected at the LHC, resulting in limits on the dark matter cross section published by the ATLAS collaboration \cite{15}.

2.3.2 Indirect detection

Indirect detection experiments try to find the standard model products of the decay and self-annihilation of dark matter particles. These products might, for example, be created in the vicinity of black holes or at the center of our galaxy, as it is expected that a large concentration of dark matter can be at found at places that have a large gravitational field. Two dark matter particles can annihilate and produce gamma rays or a standard model particle-antiparticle pair. These products can then be detected on earth. The difficult part of these experiments is the number of astrophysical objects that give a similar signal as the one that is expected from the annihilation process. Various telescopes are trying to detect emission coming from dark matter annihilation or decay. One of those telescopes is the Fermi Gamma-ray Space Telescope, which found an additional highly concentrated presence of gamma rays around the Galactic Center. This is consistent with what is expected from annihilating dark matter \cite{16}.

2.3.3 Direct detection

It is also possible to search for dark matter in direct detection experiments due to the scattering process of WIMPs. The idea behind these detectors is that they search for the scattering of dark matter particle off standard model matter within the detector. By measuring the recoil energy of the atom or nucleus, it should be possible to find the mass and cross section of the dark matter particle. Most WIMPs moving towards the Earth are expected to pass through without any interaction. However, when a detector is sufficiently large enough, the WIMPs should interact at least a few times per year with the matter inside the detector. Because of this very low interaction probability, it is essential that the background is suppressed as much as possible and that data is taken for a longer period. The interaction rate of the WIMPs with the target material in the detector can be estimated. Since the WIMPs are non-relativistic, the interaction will look like an elastic scattering with an energy transfer of typically a few tens of keV. The
interaction rate in terms of the recoil energy $E_r$, or simply the differential rate, for such interactions is given as [17]:

$$
\frac{dR}{dE_r} = N_T \frac{\rho_\chi}{m_\chi} \int_{v_{min}}^{v_{max}} \bar{\vec{v}} f(\bar{\vec{v}}) \frac{d\sigma}{dE_r} d\bar{\vec{v}} ,
$$

Equation 2.7 describes the number of expected interactions between a WIMP and a nucleus per kg detector material per day per unit deposited energy.

Figure 2.7 shows the interaction rate for a typical 100 GeV WIMP interacting with xenon, germanium, argon and neon [18]. The highest integral rate at low recoil energies is achieved using the heaviest target material xenon. In a liquid phase, such a noble gas is an excellent material to be used in a large, homogeneous and self-shielding detector. Only xenon and argon are currently used by direct detection experiments in the search for WIMPs. Argon, however, has a higher intrinsic radioactivity from $\beta$-decays, making it a disfavoured material in these low background experiments.
2.3.3.1 Exclusion limits

When a direct detection experiment fails in discovering a WIMP particle, it sets an exclusion limit on the WIMP-nucleon scattering cross section. Namely, if a WIMP would have had a WIMP-nucleon cross section above this limit, it would have been detected by the experiment. The area below this limit is unexplored parameter space where WIMPs may exist.

Figure 2.8 shows the exclusion limits and discovery claims from various experiments. The horizontal axis displays the assumed mass of the WIMP, while the vertical axis shows the achieved and projected WIMP-nucleon cross section. There are two experiments, DAMA-LIBRA (red contour) [19] and CDMS-Si (orange contour) [20], that have claimed the discovery of a dark matter signal in the past. These two discoveries however have been ruled out by exclusion limits from other experiments. The exclusion limits from XENON10 [21], SuperCDMS [22], DarkSide-50 [23], XENON100 [24], PandaX-II [25] and LUX [26] are shown in the figure. The expected limit from the XENON1T experiment after two years of running is indicated by the solid blue line, including the 1σ (green) and 2σ (yellow) sensitivity bands. The dashed blue line represents the expected sensitivity of the XENONnT experiment, the likely successor of XENON1T.

This search for WIMPs in direct detection experiments faces an encroaching background due to coherent neutrino-nucleus scattering. A large flux of solar and atmospheric neutrinos are an important background signal, as they can almost perfectly mimic an authentic WIMP signal. The more sensitive the experiments become, the harder it will be to distinguish a dark matter signal from these background neutrinos. The theoretical limit where the current experiments will lose sensitivity in detecting dark matter due to the neutrinos is represented in Figure 2.8 by the dotted orange line. Future direct detection experiments might be able to distinguish the solar neutrinos from the WIMPs by using a combination of annual modulation or directional detection [27].
Figure 2.8: Exclusion limits from several dark matter direct detection experiments [28]. The horizontal axis denotes the WIMP mass and the interaction cross section between dark matter and nucleons is on the vertical axis. Each colored band represents an exclusion limit set by a dark matter experiment. Anything above that limit is ruled out as parameter space.
CHAPTER 2. DARK MATTER
Chapter 3

The XENON1T Experiment

Direct detection experiments try to find the mass and the cross section of an incoming WIMP by measuring the recoil energy of the atom or nucleus. This energy can either be in the form of a nuclear or an electronic recoil. It is expected that WIMPs only cause nuclear recoils due to their low cross section. The goal of the experiments is therefore to discriminate a background-induced electronic recoil from a WIMP-induced nuclear recoil.

The discrimination can be performed by measuring the keV-scale recoil energy that can dissipate into three signals: heat, scintillation and ionization. The heat increases the kinetic energy of the atoms of the target, the scintillation signal is caused by emitted photons at around 1 keV/γ, and the recoil energy can ionize the atoms of the target, causing the release of free electrons at around 10 eV/γ. Note that the energies are very low compared to the energies in typical collider experiments. Therefore, the direct detection experiments use very sensitive detectors and require a very low background signal. This is the reason why the direct detection experiments are all located in underground laboratories that are well-shielded from cosmic radiation.

The detection principle that the dark matter experiments use to discriminate between the nuclear and the electronic recoils is based on one or two of the three described signals, as shown in Figure 3.1. Some dark matter searches use cryogenic crystals that detect phonon excitation (heat), combined with either ionization charge or scintillation light. Other experiments use a liquid noble gas, mostly xenon or argon, to measure the recoil energy by detecting the scintillation light and the ionization charge.

The advantage of xenon compared to argon is, among other things, that it has a higher atomic mass and that it does not have any long-lived radioisotopes that may introduce intrinsic background into the detector. It also has a high density of 2.942 g/cm³ at its boiling point of 165.05 K. This high density causes
self-shielding: background radiation depositing its energy in the outer layer of the detector medium. The energy of emitted scintillation photons is also lower than the absorption energy in liquid xenon, which makes the xenon transparent to its own scintillation light.

### 3.1 Recoil energy transfer

When a particle interacts with a xenon atom, some recoil energy is transferred to the target. The electronic recoils are mainly caused by interactions with γ-rays and β-rays, while nuclear recoils are the result of interactions with neutrons and WIMPs. These two different interactions can create a track of excited and ionized xenon atoms. The excited xenon atoms (Xe*) and the neutral atoms then form excited diatomic molecules, called excimers. When these excimers (Xe₂*) subsequently decay into the ground state, they emit scintillation light:

\[
\begin{align*}
\text{Xe}^* + \text{Xe} & \rightarrow \text{Xe}_2^* \\
\text{Xe}_2^* & \rightarrow 2\text{Xe} + h\nu \quad \text{excitation scintillation}
\end{align*}
\]  

(3.1)
The ionized atoms together with the neutral atoms form singly charged molecules. More energetic excited atoms \((\text{Xe}^{**})\) are formed when these molecules recombine with electrons. These will eventually also decay, resulting in the emission of secondary scintillation light:

\[
\begin{align*}
\text{Xe}^+ + \text{Xe} & \rightarrow \text{Xe}_2^+ \\
\text{Xe}_2^+ + e^- & \rightarrow \text{Xe}^{**} + \text{Xe} \\
\text{Xe}^{**} + \text{Xe} & \rightarrow \text{Xe}^* + \text{Xe} + \text{heat} \\
\text{Xe}^* + \text{Xe} & \rightarrow 2\text{Xe} + h\nu \quad \text{recombination scintillation (3.2)}
\end{align*}
\]

Figure 3.2 shows the process of this energy transfer. When the ionization electrons are extracted before they recombine with the xenon molecules, it is also possible to measure a charge signal \((S2)\) from the interaction. So not only the scintillation light \((S1)\) can be measured, but also the charge signal \((S2)\) when the electrons are extracted using an electric field. The fraction of these two signals differs for the electronic and the nuclear recoil interactions, making it possible to discriminate the background events from the dark matter interactions.

![Diagram of the production and collection of the S1 and S2 signals in a two-phase xenon detector](image)

Figure 3.2: Illustration of the production and collection of the S1 and S2 signals in a two-phase xenon detector [31]. Excited atoms are denoted with an asterisk.

### 3.2 Liquid xenon TPC

Detectors that use this discrimination method to find WIMPs are called liquid xenon time projection chambers (LXe TPC). They consist of a large, homogeneous volume with liquid xenon. The XENON1T detector is an example of such a detector that measures the scintillation and the ionization signal. It is a dual-phase TPC, meaning that there is a small layer of gaseous xenon (GXe) above
the liquid xenon. The electric field inside the detector is defined by multiple metal meshes. Arrays with a total of 247 photomultiplier tubes (PMTs), used to measure both the scintillation (S1) and the ionization signal (S2), are situated at the top and the bottom of the TPC. The sides of the detector are made of a highly reflective material. This causes most of the light to be reflected by the walls and detected by the PMTs. Section 3.2.1 describes the working principle of the PMTs.

Figure 3.3 illustrates the configuration of the XENON1T LXe TPC. The TPC itself is positioned in a large water tank with 84 muon-veto PMTs that act as a Cerenkov detector. When muon passes the water tank, it generates Cerenkov radiation that is detected by the muon-veto PMTs. An event in the TPC can be vetoed if there is a muon signal in the water tank at the same time. This shield reduces the neutron and γ-ray background very effectively [32].

Figure 3.3: Schematic diagram of a dual-phase liquid xenon TPC [33]. Recoil energy of a WIMP-nucleon interaction results in a scintillation signal (S1). The applied electric field along the $z$-direction then separates the electrons and drifts them through the liquid xenon towards the top of the TPC. A proportional scintillation signal (S2) occurs when the electrons emerge from the liquid xenon (LXe) to the gaseous xenon (GXe) and accelerate.
When an event occurs, scintillation light is first created by the incoming particle that interacts with the xenon. This S1 signal is almost immediately detected by the PMTs. The electric field along the $z$-direction then separates the electrons and drifts them through the liquid xenon towards the top of the detector. A second electric field extracts the electrons into the layer of gas where they are accelerated. If this acceleration gives the electrons enough energy, they create a second signal via proportional scintillation (S2), which is also detected by the PMTs. The difference in time between the S1 and the S2 signal is the drift time of the electrons. This drift time is used to measure the $z$ coordinate of the interaction. The $x$ and $y$ coordinate can be reconstructed using the hit pattern in the PMTs.

The shape of the S2 signal differs for the electronic ($\gamma$-ray, $\beta$-ray) and the nuclear recoils (neutrons and WIMPs). The S2 signal differs because the ionization density for tracks in liquid xenon is much higher for nuclear recoils than for electronic recoils [29]. The electrons are therefore more easily separated from the xenon ions in electronic recoils, resulting in a larger S2 signal. This difference in the signals is shown in Figure 3.4.

Figure 3.4: The difference in the S1 and S2 signals between a nuclear recoil event and an electronic (background) event [29].

The ratio between the S2 and the S1 signal is thus used to discriminate between electronic and nuclear recoils, and therefore between the background (electronic) events and the dark matter candidate (nuclear) events. The three-dimensional position reconstruction allows furthermore for background reduction. A WIMP interaction is namely expected to only interact once within the detector, and its distribution in the TPC volume should be uniform. However, background particles such as gammas are expected to interact at the edge of the volume due to the self-shielding property of xenon. A fiducial volume is therefore devised that consists of an inner volume inside the TPC, illustrated by the dashed red line in Figure 3.3. The nuclear recoil events that occur inside the fiducial volume are potential candidates for dark matter particles.
3.2.1 Photomultiplier tube

A PMT inside the TPC detects light at the photocathode, which then emits photoelectrons by the photoelectric effect. The photoelectrons are focused onto the first dynode, where they are multiplied with the help of secondary electron emission. This process of photoelectron multiplication is repeated at each subsequent dynode. The PMTs utilize a high voltage to accelerate the photoelectrons within the chain of dynodes. The multiplied secondary photoelectrons that are emitted by the final dynode are collected by the anode inside the PMT, which delivers the output signal. Figure 3.5 shows the operation of a PMT.

Figure 3.5: Working principle of a PMT [34]. The PMT uses a photocathode to convert photons into free photoelectrons. The photoelectrons are then accelerated in an electric field towards the dynodes. The dynodes multiply the photoelectrons, which are finally collected by the anode. The anode current is externally available and connected to charge amplifiers.

During the lifetime of XENON1T, the performance of every PMT channel is weekly verified by the PMT calibration system. The main goal of this system is to measure the gain of each PMT individually. The gain of a PMT is defined by the final amount of photoelectrons created by one induced photoelectron via one photon. It depends heavily on the voltage applied to the PMT. By regularly calculating the gain of each PMT, it is possible to correct the signals that come out of the PMTs using the appropriate gains.

The gain calibration procedure starts with a pulse generator that sends synced pulses to four individual LEDs. From each of the four LEDs, there is a fiber guiding blue light (\(\lambda = 470\) nm) to the top of the TPC. The intensity of the light is adjusted, such that the ratio of events with a PMT signal to the events with no signal is equal to 5.0%. This ratio ensures that a signal is achieved that almost exclusively consists of single photoelectrons. At the top of the TPC, each fiber line is divided into 7 fibers which are distributed symmetrically around the TPC at two different heights. The single photoelectrons are detected by the PMTs during
the gain calibration data taking. The gain is found by calculating the number of electrons produced in response to the single photoelectrons. The up-to-date gains of all PMTs are then stored in the database of XENON1T.

Besides using the LEDs to calibrate the PMTs, they can also be used to optimize the software threshold of detecting a signal. This is explained in detail in Section 5.

3.2.1.1 Long PMT signals

The response of PMTs to a single photoelectron often contains an under-amplified and delayed component in the PMT signals. This is due to the suboptimal paths that the electrons occasionally travel inside a PMT. Various PMT components from Figure 3.5 could cause this effect. First of all, the under-amplification and delay can be explained by photoelectrons that are produced at the outer side of the cathode. These photoelectrons will undergo a suboptimal acceleration due to field inhomogeneities between the outer cathode and the first dynode. Secondly, a photoelectron might skip a dynode stage, such that it is not multiplied through secondary emission. The third and most probable explanation is that there is an impedance mismatch that causes reflection. The output impedance of the amplifier is designed to be approximately 50 ohms in order to handle the high-speed signals. When an amplifier is connected to a measurement device with a cable, a 50-ohm impedance cable is preferable and the input impedance of the measurement device should be set to 50 ohms. An impedance mismatch occurs if the input impedance of the external circuit is not exactly 50 ohms. The signals will then reflect from the input end of the external circuit and return to the amplifier and reflect back from there. This might explain the under-amplified and delayed pulses. Section 6.1 describes the consequences of these longer PMT signals for the simulation and analysis software of XENON1T data, and how these components should take the longer signals into account.
Chapter 4

Processor for Analyzing XENON1T

Chapter 3 explained how signals are produced inside the detector. When these signals are detected by the PMTs, they are processed by the processor called Pax: Processor for Analyzing XENON1T. Pax searches for one- or multiple photoelectron signals, which are later classified into S1s and S2s. The software inside Pax should be optimized, such that the efficiency of detecting photon signals is increased. For example, when 5% fewer photons are found due to suboptimal software settings, it will cause a decrease of 10% in the amount of detected double-photoelectrons that can be combined into an S1. The hitfinder module inside Pax, which determines whether photoelectron signals will be labeled as a hit, should therefore be optimized. A hit is a pulse from a PMT that passes a threshold above a certain baseline. This chapter explains the data acquisition process in XENON1T and the hitfinder algorithm.

4.1 Data acquisition system

After a signal is measured by the PMTs, it is amplified and sent to the TPC digitizers. The digitizers transform the analog data into digitized data through an analog-to-digital converter (ADC). Samples that exceed a configurable amplitude threshold, the so-called self-trigger, are forwarded from the digitizers to the data acquisition system (DAQ) Reader PCs, together with the samples before and after the crossing of this self-trigger. This ensures that small surrounding S1s are captured as well. Such a block of data is called a pulse, which contains data over approximately 1 ms.

Figure 4.1 shows a schematic of the dataflow inside XENON1T. The software on the Reader PCs computes basic quantities such as the baseline and the integral of the pulse, and stores these quantities together with the data of the pulses in
MongoDB, which is a database program. It continuously stores the raw data from the Reader PCs and forwards the data to different components inside the trigger and event builder. The event builder first reads the data from MongoDB and searches for S2s, and stores the pulses around these S2s. This begins with the trigger inside the event builder that reads the start time, the PMT-number and the integral of the pulse. Based on this information it decides whether the pulse will be sent towards the workers. The workers pull the complete pulse from MongoDB and encode and compress the data. The compressed events are then sent to the writer. This last step makes sure that the pulses are correctly sorted by time and it sends the triggered events to the data storage, which builds and stores the raw events, or directly to the data processor.

The processor that analyses the raw events from the data storage is called **Pax**: Processor for Analyzing XENON. The software tool is for the greater part being developed by Nikhef and is used for doing digital signal processing of the
4.2 HITFINDER

XENON1T raw data. Figure 4.2 shows the various signal types used inside Pax. When a pulse from a PMT passes a threshold above a certain baseline, it is defined as a hit. Pax compares the gap-size between multiple hits in multiple PMTs. If the hits have a gap-size smaller than 2 µs, they are clustered into a new group, called a peak. A peak is thus a collection of hits across one or more PMTs. The peaks are then summed up and combined into a summed waveform. Various quantities such as the area, position, width and height of the peaks are calculated. Based on comparing the distributions of the various peaks in the parameter space of these quantities, two classification cuts are defined to identify whether the peak is an S1 or an S2. The identified peaks form the S1/S2 pairs as stated in Section 3.2. If a peak falls in between the two classification cuts, it is labeled as an unknown peak.

![Figure 4.2: Signal types used inside Pax](image)

Figure 4.2: Signal types used inside Pax. Pulses that pass a threshold are defined as a hit. Hits in the same time domain are combined into peaks. Based on its properties, the peak is labeled as an S1, S2 or unknown signal.

### 4.2 Hitfinder

The first step of Pax is determining whether there is a hit (or multiple hits) inside a pulse. The module inside Pax that is responsible for this task is called hitfinder. The hitfinder first calculates the baseline of the pulse, which is defined as the mean of only the first 40 samples in the pulse. This insures that the height of the hit itself is not included in the calculation of the baseline. The hits are then found based on an upper and boundary threshold. The boundary threshold, explained in more detail in Section 6, determines where the hit starts and ends, while the hit has to pass the upper threshold somewhere between this start and endpoint.

An example of a pulse with a hit is shown in Figure 4.3. It shows a single photon hit that is simulated on top of XENON1T noise data. The horizontal axis displays the time, where each sample number is equal to 10 ns. The vertical axis denotes the amount of the light that comes from the PMT, either in ADC counts (left) or in photoelectrons per sample (right). The photoelectron (pe) is a unit of electric charge. One photoelectron is defined as the total amount of charge of one emitted photoelectron. The height of the upper threshold (red dashed line) and the boundary threshold (green dashed line) in the example are determined by the height of the noise level (dotted gray line) in the pulse. The noise level σₙ is
defined in each pulse as the root mean square deviation from the baseline:

$$\sigma_n = \sqrt{\left< (w - \text{baseline})^2 \right>} ,$$

(4.1)

where \(w\) is the height of a sample. The average in the equation only runs over the samples that are lower than the baseline. The lower and the upper threshold can be defined as a multiple of this noise level, named the height-over-noise ratio. The upper threshold in Figure 4.3 is set at a height-over-noise of 7, which means that it is fixed at 7 times the noise level \(\sigma_n\). This is very conservative since most single photoelectron (SPE) pulses have heights of more than 15 times the noise. The boundary threshold is set at 3 times the height-over-noise.

The height of the upper thresholds and boundary threshold could also be based on other quantities than the height-over-noise parameter, such as the width of the hit or the area of the hit. However, as shown in Section 5.2, the height-over-noise parameter is the most suitable parameter to optimize the hitfinder algorithm.

Sometimes the hits show longer tails. The boundary threshold is therefore raised by a fraction of the height of the hit after a hit has been found. After the pulse has ended, the boundary threshold is set back to its defined level. Section 6.1 further examines these longer tails and its impact on the hitfinder algorithm.
Chapter 5

Upper Threshold Optimization

Whether the hitfinder module in Pax labels a certain pulse as a hit depends on the upper threshold. The algorithm that determines the height of this upper threshold must be optimized such that the hitfinder finds as many one- or multiple photoelectron signals as possible, while it triggers as few as possible when there are no photons. This is done using a similar kind of approach as has been used in optimizing the threshold for the XENON100 detector, the predecessor of XENON1T [36].

5.1 PMT gain calibration

The upper threshold is optimized using data from the PMT gain calibration procedure. This procedure is explained in detail in Section 3.2.1. The data from the PMT gain calibration consists of noise-only data when the LED is turned off, and data with photon pulses when the LED is turned on. The data is processed with Pax using an upper threshold of three times the noise. The optimal threshold is found by estimating and comparing the acceptance rate and dark hit rate for multiple upper thresholds (larger than three times the noise). Figure 5.1 displays the hit rate per PMT in this data. After approximately 0.4 $\mu$s, the LED is turned on for 0.2 $\mu$s. It is striking that the hit rate is higher before the LED is turned on than after it is turned off. It could be that some of the PMTs are over-saturated due to the intensity of the LED signal, however this should be further investigated.

It might be better to use PMT gain calibration data where the LED is turned on for a longer period since that would increase the amount of data with photon pulses. Unfortunately, the LED is turned on only for short periods to calibrate the gains of the PMTs. Nevertheless, it will turn out that this data has sufficient statistics to optimize the upper threshold.
CHAPTER 5. UPPER THRESHOLD OPTIMIZATION

Figure 5.1: Logarithm of the mean hit rate per PMT in the LED dataset as a function of time. The LED is approximately turned on at 0.4 μs for a duration of 0.2 μs.

With these data, it is possible to define a region where the LED is turned off, hence where only dark hits exist. The hits found in this region come for example from thermal emission from the photo-cathode in the TPC. The dark hit rate (in Hertz per PMT) for a particular upper threshold can be calculated. Based on Figure 5.1, the dark region is defined as the period between 1 μs and 2 μs. A second region that can be defined is the light region, which contains mostly photon hits. This will be the time period where the LED is turned on. The light region is in this dataset defined as the period between 0.4 μs and 0.6 μs. The LED hits in the light region will also contain some noise and hits from the dark rate. The main goal will be to subtract the noise and dark rate from the true photons. After that step, it will be possible to estimate the hitfinder acceptance rate of the light hits for various upper thresholds, together with the corresponding dark rate.

This can only be done for PMTs that are actually working. The PMTs in the detector that are malfunctioning should not be included in the analysis. By plotting the hit rate in the light region for each PMT separately, as has been done in Figure 5.2a and 5.2b, it is possible to see which PMTs are dead. The dead PMTs are the ones with a low hit rate, indicated by the blue and white background color. The cutoff is set at 10^3 Hertz, such that PMT number 1, 12, 26, 34, 65, 86, 88, 130, 135, 137, 148, 152, 176, 188, 198, 206, 213, 214, 234 and 244 are excluded from the analysis. The hit rate is higher for the bottom PMTs compared to the top PMTs because the LEDs are targeted towards the bottom PMTs.
5.2 Discrimination parameters

After excluding the bad PMTs from the analysis, it is possible to test whether the height-over-noise parameter that the hitfinder uses to detect hits is actually a sufficient parameter to discriminate LED hits from dark hits. This is verified by calculating the amount of LED hits and dark hits in the LED dataset using different parameters to define the upper threshold. The discrimination parameters that the height-over-noise parameter is compared with are based on the hit properties that Pax calculates when it analyses a hit. These are the absolute height (in ADC counts), the area, the area-over-noise and the width of the hit. The area-over-noise is defined as the area of the hit divided by the noise level $\sigma_n$, which is calculated using Equation 4.1. The width of the hit is the time between the start and the endpoint of the hit.

Figure 5.3 shows the result of the comparison between the five discrimination parameters. The numbers denote the thresholds used by the corresponding discrimination parameter at those specific points. The threshold is given in pe for the area, pe/bin for the height and in ns for the width of the hit. Due to the intrinsic time-resolution of the digitizers, the width is always a multiple of 10 ns. The parameter with the best discrimination power should pass the most LED hits for a given dark rate, which corresponds to the highest line in Figure 5.3. This means that the height-over-noise and the area-over-noise parameter perform better than the area, width, and height in discriminating LED hits from dark hits. The data
has already been processed with Pax using a height-over-noise threshold of three. Hence, hits with a height just above the noise level are already removed from the data, while these hits would have been easy to eliminate by the hitfinder height-over-noise threshold. This makes the comparison between the area-over-noise and the height-over-noise biased since the height-over-noise actually performs better than suggested by the graph. The height-over-noise is therefore chosen as the most suitable measure to discriminate LED hits from dark noise hits.

![Figure 5.3](image.png)

Figure 5.3: The ability of five different hit properties used as the upper threshold to discriminate LED hits from dark hits in the LED dataset. The numbers in the figure denote the thresholds used by the corresponding discrimination parameter at those specific points.

### 5.3 Optimal height-over-noise ratio

The next step is to obtain a first insight into the range where the upper height-over-noise threshold should approximately be set. This is done by plotting the area and the height in terms of the noise level for each hit separately. Figure 5.4a shows the area (vertical axis) versus the height (horizontal axis) for each LED hit, while Figure 5.4b displays the area versus height for the dark hits. Both figures indicate that all the hits with a height lower than three times the noise level have already been cut by Pax, as mentioned in the previous section.
5.3. OPTIMAL HEIGHT-OVER-NOISE RATIO

Hitfinder will reject all the hits that have a lower height-over-noise ratio than the upper threshold. The bulk of dark hits in the lower left corner of Figure 5.4b should probably be rejected since those hits are probably noise hits because of their low hit area. This rejection can be achieved by taking an upper threshold of at least four times the noise. However, a thorough analysis is needed to determine the optimal height for the upper threshold more precisely.

Figure 5.4: The area and the height-over-noise of each hit in the LED dataset. Both figures indicate that all the hits with a height lower than three times the noise level have already been cut out by Pax.

The more accurate optimization of the upper threshold starts with plotting the distribution of the LED hits and the dark hits at various height-over-noise parameters, shown in Figure 5.5. Many extra hits are found with a height-over-noise parameter lower than approximately 12 due to the noise that is present. It is impossible to determine the amount of noise in this region and to distinguish it from the real LED hits. The number of real hits in the region below 12 times the height-over-noise can however be estimated by extrapolating the LED hit distribution in the region that is much less affected by the noise. This extrapolation (dashed blue line below 12 times the height-over-noise) is based on a Gaussian fit that is truncated at 0 (solid blue line). The Gaussian is fitted in a limited fit range between a height-over-noise ratio of 12 and 50. The fit does therefore not correctly describe the number of hits with a height-over-noise larger than 50. However, this can be neglected since all relevant optimal values for the upper threshold have a much lower height-over-noise ratio.

The dependence on the upper threshold of the hitfinder acceptance of LED hits can be calculated using the extrapolated distribution for the hit height-over-noise.
This acceptance is calculated using the extrapolated hit distribution in the region below a height-over-noise ratio of 12 and the solid black line for higher ratios. Another approach would be to only use the extrapolated hit distribution (blue line) to calculate the acceptance of LED hits, instead of the black line. However, as it is not known how good the Gaussian fit approximation is, it is best to use the data for the height-over-noise ratios larger than 12.

Figure 5.5: Distribution of hits in the height-over-noise parameter while the LED is turned on (black) and the LED is turned off (purple). The Gaussian fit, denoted by the solid blue line, is fitted in the region between 12 and 50 times the height-over-noise. The dashed blue line is the extrapolation of the fit.

The estimated LED hit distribution in Figure 5.5 allows to display the relation between the acceptance of the hitfinder and the upper threshold. Furthermore, the hit rate of the dark hits for each upper threshold can be determined directly from the dark hit data. So the hitfinder acceptance of the LED hits, as well as the dark hit rate, can be plotted for various upper thresholds, which is exactly what is needed to optimize the upper threshold. This relation is shown by the blue line in Figure 5.6.

It displays that the requirement of finding as many LED hits as possible (a large hitfinder acceptance) with a minimum amount of dark hits results in an optimal upper threshold between four and five times the noise level. A threshold lower than four times the noise results in a significant increase in the dark hit rate.
and only a small gain in the number of accepted photons. On the other hand, an upper threshold larger than five times the noise results in a large loss of photon detection, while the dark hit rate decreases only slightly. Thus an upper threshold of around 4.5 is optimal, which is in correspondence with the first estimation that was based on Figure 5.4.

## 5.4 Self-trigger

So far, it has not been taken into account that before normal data (not PMT gain calibration data) is analyzed by Pax, it already passes a certain threshold that is set by the digitizers. This self-trigger in the digitizers, as explained in Section 4.1, ensures that only the regions around outliers larger than 15 ADC counts are recorded and digitized, resulting in a significant amount of data reduction. The self-trigger in the digitizers thus cuts a lot of pulses that have a low ADC count. All the PMT gain calibration data used in this optimization, however, is taken without the self-trigger in the digitizers. This implies that a lot of the photoelectrons that are hidden in the noise in the analysis would normally already have been removed by the self-trigger. The blue line in Figure 5.6 should thus be revised, such that only hits that would pass the self-trigger of 15 ADC counts are analyzed. The green line in Figure 5.6 displays the acceptance of the hits that would also have passed the 15 ADC counts threshold that is normally set by the digitizers.

Figure 5.6 shows that without the self-trigger, the hitfinder is not able to find approximately 1% to 3% of the LED hits due to the photoelectrons that are hidden in the noise signal. They can only be found by the hitfinder if the upper threshold is set at a very low value, however, that would also increase the dark rate, as indicated by the blue line.

However, when the self-trigger of 15 ADC counts is applied, most of these problematic photoelectrons have already been cut away before they reach the hitfinder module in Pax. The self-trigger also automatically causes the dark hit rate to decrease, since a lot of those hits have a height that is lower than 15 ADC.

Looking at the hitfinder efficiency for hits after the self-trigger in Figure 5.6 (green), it follows that as long as the upper threshold is chosen somewhere between 3 and 6 times the noise, the acceptance of the hitfinder after the 15 ADC self-trigger threshold will almost be equal to 1. Furthermore, the amount of dark rate will not change by a compelling amount for different upper thresholds in that range. Therefore, the upper threshold can be set to a value of for example 6 times the average noise level. For this upper threshold, the hitfinder will find as many one- or multiple photoelectron signals as possible, while it triggers almost never when there are no photons.
Figure 5.6: The acceptance of the hitfinder and the dark hit rate plotted for various upper thresholds, indicated in units of the noise level $\sigma_n$. 

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Chapter 6

Lower Threshold Optimization

The second threshold that is revised is the boundary threshold. The boundary threshold sets the start and endpoint of each hit. The hit starts when the pulse crosses the boundary threshold for the first time and stops when it passes the boundary threshold for the second time. The height of the boundary threshold thus determines the area of the hit by setting the start and endpoint. A higher boundary threshold corresponds to a lower area because in that case the start and endpoint are located closer to each other. Similarly, a lower boundary threshold corresponds to a higher area for the hit and also a higher variance due to the extra noise that is integrated. Figure 6.1 illustrates the dependence of the area and the boundary threshold, by integrating the same pulse using two different boundary thresholds, resulting in two two different hit areas. The boundary threshold is also made dynamic in the sense that it is temporarily raised to a fraction of the hit height after a hit has been encountered. This prevents the integration of long tails that are present in some pulses. However, as Section 6.1 shows, this dynamic component results in a large bias in the integration of the hit area.

Single photon hits are used to optimize this threshold. Single electrons consist of hits that are almost always caused by single photons. The expected mean area of these hits should thus also be equal to exactly 1 photoelectron (pe). In real data, however, the average hit area is found to be a little higher than this 1 pe because of two main aspects. First of all, the ultraviolet photons from liquid xenon can cause some double-photoelectron emission from the photocathode of the PMTs [37]. Additionally, detection of the photoelectrons for smaller pulses is harder due to the thresholds set by the self-trigger and the hitfinder. These two factors increase the average area to slightly above 1 pe in real data.
CHAPTER 6. LOWER THRESHOLD OPTIMIZATION

(a) Boundary threshold of 10 ADC.

(b) Boundary threshold of 3 ADC.

Figure 6.1: Integration of the same hit using two different boundary thresholds. The boundary threshold of 3 ADC counts results in a larger hit area compared to the 10 ADC counts boundary threshold.

Therefore, simulated data instead of real data is used to optimize the boundary threshold, since that allows to create photons with an average hit area equal to 1 pe. The simulation consists of 100,000 S1 single photons released in the TPC. It also emulates the response of the PMTs and the digitizers to the simulated photons. The following steps occur in the simulation:

1. The arrival time of the photon signal in the PMT is calculated

2. Up-to-date PMT gains are fetched from the XENON1T database (as described in Section 3.2.1)

3. Based on the photon arrival time, it is determined in which digitizer bin the photon signal is to fall.

4. The charge deposited in each bin is computed and converted to ADC counts

5. The ADC charge of several digitizer bins close to the signal center are combined into a single pulse

6. Real noise data is added for each PMT separately

7. The pulse is added to an initially empty waveform, at the correct time value
This process is repeated for each PMT. Even for the PMTs that receive no photons, as they will still measure the noise. Finally, the waveforms for all PMTs are combined into a \texttt{Pax} event object that can be processed further. Because each arrived photon is in the simulation is treated separately and independently, PMT saturation effects are ignored. At the end, the waveforms for all PMTs are combined into a \texttt{Pax} event object that can be processed further.

The boundary threshold must be set such that the simulated single photon hits have an average hit area as close to 1 pe as possible, combined with an as low as possible variance in these areas. Figure 6.2 shows this variance set out against the bias for the simulated single photoelectron hits. The bias is defined as the difference between the expected average hit area of 1 pe and the average hit area found in the simulation.

![Figure 6.2: Variance and bias in the average hit area for various boundary thresholds. The numbers on the line denote the height of the boundary threshold (in ADC counts) at those specific points.](image)

The optimal value for the boundary threshold should correspond to a low bias and a low variance. Namely, when these two factors are minimized and evaluated, it is possible to use the mean area per hit in single electrons to quantify the double-photoelectron emission probability. Unfortunately, there is no boundary threshold that results in both the lowest bias and the lowest variance. Besides that, it is hard to weigh a low bias against a low variance. Based on the plot it can therefore only be concluded that a suitable boundary threshold should be set at a level between 1 and 11 ADC, for example at 6 ADC. Boundary thresholds higher than 11 ADC counts are always suboptimal, as there is always another boundary threshold that results in a smaller area bias and a smaller variance.
6.1 Long-tailed pulses

The waveforms from the previous section have been simulated using a double-exponential photoelectron pulse model, such as the simulated pulse in Figure 4.3. The simulation ignores the effect of under-amplified photoelectrons inside a PMT that can cause long tails in pulses, as explained in Section 3.2.1.1. This can lead to a bias in the mean area of the hits up to 20% [38]. For large signals, this is less of a problem since they do get fully integrated due to the many hits that pile up. However, for the smaller signals this under-amplified component should be taken into account, else it could lead to a non-linearity in the energy scale of the signals.

A new photoelectron pulse model is therefore made that does contain the long pulse tails. This model is based on the median normalized waveform of real single photoelectron hits. It is created by selecting the hits that constitute single electrons. For each hit, the PMT waveform is taken that the digitizer recorded around that hit. The waveforms are then aligned based on their maximum amplitude. At each sample, the median amplitude is taken over all the waveforms. This median amplitude is shown in Figure 6.3. An example of a pulse created with this new waveform model, simulated on top of XENON1T noise data, is shown in Figure 6.4.

![Figure 6.3: The median PMT waveform around hits found in single electrons [36]. It is created by taking PMT waveforms that the digitizer recorded around single electron hits. These waveforms are then aligned based on their maximum amplitude. At each sample, the median amplitude is taken over all the selected waveforms.](image)
6.2. IMPROVED HITFINDER ALGORITHM

Currently, the boundary threshold in the hitfinder is temporarily raised to a fraction of the hit height after a hit has been encountered. This prevents the tails from being integrated by the hitfinder module in Pax, as the pulse in Figure 6.4 clearly shows. The tails should however not be ignored since that could lead to the non-linearities in the energy scale. Figure 6.5 shows how the performance of the hitfinder becomes worse for the long-tailed pulses that are simulated with the new photoelectron pulse model. The area bias increases by 20% compared to the hitfinder applied on the former double-exponential photoelectron model that does not show the long tails, while the variance also rises. The hitfinder algorithm must thus be improved such that the long-tailed pulses get fully integrated.

6.2 Improved hitfinder algorithm

An improved and simpler hitfinder algorithm is created to integrate the long-tailed pulses. A hit is still found when a pulse exceeds the upper threshold, however, the dynamic boundary threshold that determined the integration bounds in the previous hitfinder no longer exists. The domain over which the pulse is integrated is defined by a fixed amount of time before and after the hit passes the upper threshold. This amount of time is called the left-extension for the left integration.
CHAPTER 6. LOWER THRESHOLD OPTIMIZATION

Figure 6.5: Variance and bias in the average hit area for various boundary thresholds. The integration performance of the hitfinder applied on the former pulse model without long-tailed pulses (blue) is a reproduction of Figure 6.2. The integration of the new pulse model that does include long-tails (green) results in a larger area bias and variance, due to the ignorance of the long-tailed pulses by the hitfinder integration algorithm. The numbers in the figure denote the height of the boundary threshold (in ADC counts) at those specific points.

The tail is integrated as well due to the improved hitfinder algorithm. This also causes the increase in hit area, compared to the area that was found in Figure 6.4 using the previous hitfinder. The question that arises is what the optimal values are for the left-extension and the right-extension. For the first science run of XENON1T, that started in November 2016 and ended on January 2017, the default setting was a left-extension of 30 ns and a right-extension of 200 ns. These two bounds should however be extended to such an amount that the whole hit including the tail is integrated, without increasing the variance caused by the additional integration of noise. The same method as in optimizing the boundary threshold for the previous integration algorithm is used.
6.2. IMPROVED HITFINDER ALGORITHM

Because the long-tailed pulses still arise from single photoelectrons, it is expected that their average hit area is equal to 1 pe. The left-extension and right-extension should thus be set such that the simulated photons have an average hit area close to 1 pe, together with an as low as possible variance in the area. This optimization is performed using a simulation of 100,000 S1 single photons. The simulation is similar to the one used in optimizing the boundary threshold from the previous hitfinder algorithm, explained at the beginning of this chapter.

It can happen that a PMT emits two photoelectrons when struck with only one photon of sufficiently high energy. That would increase the expected area to a higher level than 1 pe due to the creation of two photoelectrons. To prevent this, the probability of double photoelectron emission is set to zero.

The areas of all the hits inside the simulated pulses are calculated. Figure 6.7 shows the variance in these areas set out against the area bias (which is defined as the difference between the average hit area and 1 pe), for various integration bounds. The left and right plot display the optimization of the left-extension and right-extension, respectively. Note that these two bounds are always set as a multiple of 10 ns due to the constrained resolution in the digitizers.
CHAPTER 6. LOWER THRESHOLD OPTIMIZATION

(a) Left-extension optimization.

(b) Right-extension optimization.

Figure 6.7: (a) Variance and bias in the average hit area for various integration bounds for the optimization of the left-extension. (b) The same as (a), but for the optimization for the right-extension. The numbers in the plots denote the bounds used at those specific points. The integration bounds used in the first science run are denoted by SR0. The left-extension is optimized using a right-extension of 150 ns, while the right-extension is optimized using a left-extension of 10 ns.

The optimal left-extension and right-extension correspond to the lowest area bias combined with the lowest variance. The left plot in Figure 6.7 indicates that this clearly coincide with 10 ns for the left-extension. This differs from the 30 ns that have been used in the first science run of XENON1T. For the right-extension on the right plot, it is harder to pick an optimal value since each value between 150 ns and 200 ns either has a lower bias or a lower variance. The right-extension of 200 ns that was used in SR0 corresponds to the lowest area bias, however, a lower variance can be achieved if it is lowered to 150 ns.
Chapter 7

Bayesian Inference

Over the last few decades, many physics experiments have searched for new particle productions, particle reactions or particle decay modes. They try to find new physical laws that are not incorporated in the Standard Model of Particle Physics. Most of these experiments do not succeed in making claims of new physics, and instead, report upper limits on the rates of the hypothetical particles.

The upper limit on the WIMP-nucleon scatter cross section of the XENON1T experiment depends on the background prediction and the conversion from the deposited energy inside the detector into observable signals, which is partly performed by the hitfinder algorithm from the previous chapters. The profile likelihood analysis is the statistical method that is commonly used to calculate the upper limit for dark matter experiments, including the XENON1T experiment. This analysis draws conclusions from data by emphasizing the frequency of the observed data in hypothetical similar experiments. This is sometimes referred to as frequentist statistics, which is introduced in the first section of this chapter. Subsequently, Bayesian inference is introduced as an alternative method to determine the upper limit of the XENON1T experiment. This method allows combining past knowledge with current experimental data to set an alternative upper limit.

7.1 Frequentist statistics

For the XENON10 experiment, the predecessor of XENON100 and XENON1T, the maximum gap method was used to set an upper limit. As the name suggests, this method finds the best gap between events for setting an upper limit, which is explained in detail in [39]. The profile likelihood technique has been introduced in the dark matter research by the XENON collaboration as an alternative method to set an upper limit for the XENON100 experiment [40]. This technique allows
to include systematic uncertainties from the background and signal models in a frequentist framework.

In frequentist statistics, probabilities are treated as long run relative frequencies. The performance of statistical tests in frequentist statistics is determined by an infinite amount of hypothetical repetitions of the experiment. The parameters of interest in a specific model, which are the WIMP mass and the WIMP-nucleon cross section for the XENON1T experiment, are considered as fixed but unknown constants. Because they are treated as constants, it is meaningless to make a statement about the probability distribution of the unknown parameters.

It is however possible to test a specific hypothesis using experimental data. For setting the upper limit on WIMP-nucleon cross sections, it is tested whether the data from the detector shows only background ($\sigma = 0$, null hypothesis $H_0$) or that it displays a signal on top of the background ($\sigma > 0$, signal hypothesis $H_\sigma$). The test statistic $t$ that reduces the observed data to only one value and tests these two hypotheses against each other is given as [41]:

$$t = \begin{cases} 
-2 \ln \left( \frac{L(\sigma; \hat{n}_j)}{L(\hat{\sigma}; \hat{n}_j)} \right), & \text{if } \sigma \geq \hat{\sigma} \\
0, & \text{if } \sigma < \hat{\sigma}
\end{cases} \quad (7.1)$$

Here, $L$ is the likelihood function that is described in more detail in Section 8.1. The parameters $n_j$ are nuisance parameters, and rely on the attempt to divide the likelihood function into components representing knowledge about the parameters of interest and information about the other (nuisance) parameters. The parameters $\hat{\sigma}$ and $\hat{n}_j$ are the maximum likelihood estimators (MLE) that maximize the likelihood for the current set of data, and $\hat{n}_j$ is the conditional MLE obtained for the nuisance parameters at the fixed value of $\sigma$ under test. In frequentist statistics, the nuisance parameters are thus taken care of by taking the values that maximize the likelihood. The test statistic $t$ is set to zero for $\sigma < \hat{\sigma}$ because, when setting an upper limit, data with $\sigma < \hat{\sigma}$ should not be regarded as representing less compatibility with $\sigma$ than the data obtained, and therefore this is not taken as part of the rejection region of the test.

A larger value of $t$ in Equation (7.1) corresponds to a greater incompatibility between the tested hypothesis and the data, indicating that the dark matter signal hypothesis is false. Rejecting the background-only hypothesis is only a part of discovering a WIMP. The possible existence of WIMPs when the signal hypothesis is true also depends on the interpretation of the physical origin of such a signal.

Following the procedure described in [40], the frequentist upper limit is calculated as follows. Let $f(t|H_\sigma)$ be the probability distribution function of the test statistic $t$ under the signal hypothesis $H_\sigma$, and let $t_{\text{obs}}$ be the value of the test statistic obtained with the experimental data. The signal p-value $p_s$ is defined as the probability that the outcome of a hypothetical, identical XENON1T experiment results in a test statistic larger than the observed one, while the signal
hypothesis \( H_\sigma \) is true. Therefore, \( p_s \) is given by

\[
p_s = \int_0^\infty f(t|H_\sigma) dt.
\]

(7.2)

According to frequentist statistics, the signal hypothesis \( H_\sigma \) has to be rejected with 90% confidence level (CL) if \( p_s \leq 10\% \). The 90% CL upper limit \( \sigma_{\text{up}}(m_\chi) \) on the cross section \( \sigma \) for a given WIMP mass \( m_\chi \) is therefore found by solving

\[
p_s(\sigma = \sigma_{\text{up}}(m_\chi)) = 10\%. \tag{7.3}
\]

According to Wilk's theorem, the distribution for the test statistic \( t \) in Equation (7.1) is a \( \chi^2 \) distribution in the limit of large samples [42]. This chi-square approximation is used in Equation (7.2) in order to estimate the signal p-value \( p_s \).

The frequentist upper limit should be interpreted as: no matter what the true value of \( \theta \) is, if a hypothetical group of similar experiments measure \( \theta \) and construct their 90% CL upper limit, then in the limit of a large ensemble of experiments, 90% of the confidence regions (the region below the upper limit) contain the unknown true value of \( \theta \). This property of is called coverage. Frequentist statistics thus tends to say more about the probability of observing a similar upper limit in future dark matter experiments with the same expected signal and background, than about the non-existence of the signal itself.

The frequentist statistical approach is objective in the sense that it disregards any prior knowledge regarding the process being measured. However, in the dark matter research, there is prior knowledge about the parameters of interest. Previous experiments have already set upper limits, and it can be seen as a waste of information if this knowledge is not used. In addition, there are various supersymmetry (SUSY) models that favor the existence of WIMPs at specific parameter ranges, as discussed in Section 8.5. Since it is not possible to use this prior information in frequentist statistics, an alternative statistical approach is proposed to set an upper limit for the XENON1T experiment in which prior information can be included in the analysis.

### 7.2 Bayes’ theorem for parameter estimation

Bayesian inference is a statistical approach in which prior knowledge can be used. It combines prior knowledge about the process with the experimental information about the process that is contained in the data. This results in a posterior probability. The prior beliefs on the parameters are revised based on the experimental data by using Bayes’ theorem. Bayesian inference allows for direct probability statements about the unknown parameters since the parameters are considered as random variables due to the uncertainty about their true value.
This alternative approach to statistics gives a consistent method to update the beliefs about the unknown parameters by observing the data. The inference is based on the measured data, instead of all possible datasets that might have occurred, as happens in frequentist statistics. To obtain the joint distribution of only the parameters of interest, the nuisance parameters are taken care of in Bayesian inference by integrating them out, which is called marginalization.

The result of Bayesian inference is the posterior probability, which is the probability density (or beliefs) of the parameters $\theta$ after incorporating the data $d$ of the experiment. It is determined by invoking Bayes’ theorem, which describes how the probability distributions of the parameters in the model change after the information in the data is taken into account. The posterior distribution is given by

$$ P(\theta|d) = \frac{\pi(\theta) \cdot L(d|\theta)}{\int \pi(\theta) \cdot L(d|\theta) \, d\theta}. \quad (7.4) $$

The posterior is thus proportional to the initial probability density function for the parameters $\pi(\theta)$ (the prior), multiplied by the distribution of the observed data conditional on its parameters (represented by the likelihood $L(d|\theta)$). The prior reflects the beliefs on the parameters before the experiment is performed, and is discussed in more detail in Section 7.3. The posterior distribution is found after this multiplication is normalized by the integral of the likelihood times the prior over all possible parameter values, as shown in the denominator.

### 7.3 Prior distribution

A commonly used prior in particle physics is the uniform prior, which assigns an equal probability to all possible values of the parameters. The problem that arises however is in which quantity the prior should be uniform, such that it is invariant under transformations of the parameter. It could be uniform in linear space, in log-space, or in any other metric. Each choice for a specific metric affects the posterior distribution. The fact that the posterior distribution depends on this non-objective choice is one of the reasons why Bayesian inference appears inconvenient to many frequentist analysts.

The main dilemma for Bayesian inference is therefore to argue in what metric the prior should be uniform. The two most common choices for uniform priors in the dark matter search are the flat-prior and the log-prior [43]. The flat-prior is uniform in linear space and is defined as:

$$ \pi_{\text{flat}}(\theta) = \begin{cases} 1, & \text{if } \theta_{\text{min}} \leq \theta \leq \theta_{\text{max}} \\ 0, & \text{otherwise.} \end{cases} \quad (7.5) $$
Again, $\theta$ represents the parameters of interest. The limits $\theta_{\text{min}}$ and $\theta_{\text{max}}$ define the nonnegative part of the prior and the parameter region of interest. The flat prior does not favor any subspace inside that region in particular, which is especially useful when the general order of magnitude of the parameter is known. The parameter can then take any value on this region with an equal prior probability. However, when the order of magnitude is unknown, the log-prior is more appropriate. It assigns an equal prior probability at each order of magnitude. It is defined as:

$$
\pi_{\text{log}}(\theta) = \begin{cases} 
1/\theta, & \text{if } \theta_{\text{min}} \leq \theta \leq \theta_{\text{max}} \\
0, & \text{otherwise.} 
\end{cases} \quad (7.6)
$$

As argued in [44], Bayesian inference should not depend on the parameterization of the model. This is the case for the log-prior, since it is invariant under changes of the power of the parameter of interest. Namely, the priors $\pi_{\text{log}}(\theta)d\theta = d\theta/\theta$ and $\pi_{\text{log}}(\theta^n)d\theta^n = d\theta^n/\theta^n$ are consistent for any power $n$. Both priors are proportional to $d(\ln \theta)$, which implies that the prior is uniform in the metric $\ln(\theta)$.

When there is much data available, the likelihood function is sharply peaked, and varying the assumptions in the prior distributions will have less effect on the posterior distribution. However, when there is not that much data available, the choice of the prior and the prior limits $\theta_{\text{min}}$ and $\theta_{\text{max}}$ can significantly affect the posterior distribution. This can make an objective interpretation of the Bayesian results rather difficult. It is therefore best to perform an analysis on the dependence on the priors: comparing the posterior distributions under different reasonable choices of prior distributions. The Bayesian result is robust if approximately the same posterior distribution is found for different assumptions in the prior. However, when the posterior distribution differs substantially for various priors, there is only a little that can be confidently inferred from the Bayesian inference. In that case, the results rely too heavily on the details in the prior, which might not be well chosen. The analysis on the priors for the XENON1T experiment is performed in Section 8.4.

### 7.4 Bayesian upper limit

The parameters of interest in the search for WIMPs are the mass of the WIMPs, $m_\chi$, and the WIMP-nucleon scattering cross section $\sigma$. The true value of the mass and the cross section could take on any value in the range of several orders of magnitude. Because the log-space is also commonly used as the metric to present the regions where WIMPs are excluded, as illustrated by the published upper limits in Figure 2.8. Therefore, it seems reasonable to assume the log-prior from Equation 7.6 for both parameters.
The mass and the cross section are not allowed to become negative. These two physical constraints are easily implemented in Bayesian inference by incorporating it into the prior. For the log-prior, this is automatically established since the logarithm of a negative number is undefined. For the flat prior, the constraint (or prior information) that the WIMP mass is nonnegative, is easily established by taking the prior that is zero if $m_\chi < 0$ and uniform otherwise. The physical constraint on the mass thus sets a lower limit on the value for $m_{\chi, \text{min}}$ in Equation 7.5. This applies in the same way for the cross section.

Once the prior and the likelihood are specified, the Bayesian 90% CL credible region is determined by obeying the following criterion:

$$\int_{\theta_1}^{\theta_2} P(\theta|d) d\theta = 0.90$$

where $\theta$ represents the WIMP mass $m_\chi$ and the WIMP-nucleon cross section $\sigma$, and where $P(\theta|d)$ is the posterior distribution as stated in Equation 7.4. The 90% credible region should be interpreted as that there is a 90% probability that the true value of $m_\chi$ and $\sigma$ lies inside the credible region.

Numerically, the 90% credible region is obtained by first dividing the $\{m_\chi, \sigma\}$-subspace into pixels. The posterior from Equation 7.4 is calculated at each pixel, using values for $m_\chi$ and $\sigma$ that correspond to that pixel. The posterior values are then sorted by value. The pixels that correspond to the lowest posterior values that together sum up to 90% of the total sum of all posterior values, are contained in the 90% credible region. If the credible region contains the pixels for which $\sigma = 0$, the Bayesian upper limit is the line that demarcates the 90% credible region.

The Bayesian upper limit for XENON1T should be interpreted as that there is a 90% probability that the true value of $m_\chi$ and $\sigma$ lies in the region below the upper limit. Note that this interpretation differs from the frequentist interpretation of the upper limit from Section 7.1. The requirement of frequentist coverage does therefore not apply (and is in general not fulfilled) in the context of Bayesian inference, where the credible region is obtained by integration of the posterior distribution. This makes it hard to draw conclusions from the comparison of frequentist upper limits and Bayesian upper limits.
Chapter 8

Bayesian Upper Limit for XENON1T

So far, most dark matter experiments have reported upper limits on the WIMP-nucleon cross section as a function of the WIMP mass. These published upper limits are usually calculated with frequentist statistics. This has also been the case for the 90% CL upper limits that were reported by the dark matter experiments XENON100 and XENON1T. As shown in the previous chapter, such an upper limit differs from the upper limit that is calculated with Bayesian inference. In this chapter, the Bayesian upper limit on the WIMP-nucleon cross section is calculated using XENON1T’s first science run results and compared with the frequentist upper limit. This is possibly after the XENON1T likelihood function is specified.

8.1 Likelihood function

The fundamental quantity for Bayesian inference and frequentist statistics is the likelihood function $L$. It measures the extremeness of data under the hypothesis. In Bayesian inference, it relates the posterior and the prior distribution. Direct detection experiments do not make their likelihood functions generally available. Nonetheless, the general form of the likelihood function from the XENON1T experiment is known and given as

$$
\ln L = -\mu + \sum_{i} \ln \left( \sum_{j} \mu^{(j)} \text{PDF}^{(j)}(\text{event}_{i}) \right). \quad (8.1)
$$

Here, $\mu$ is the expected number of events for seven different event sources inside the detector, $\mu^{(j)}$ is the expected number of events for source $j$, and $\text{PDF}^{(j)}$ is the probability density function of the events from source $j$. As described in detail
in [45], these seven sources are WIMPs, electronic recoils (ER), radiogenic neutrinos, coherent neutrino-nucleus scattering (CNNS), accidental coincidences, wall leakage events, and anomalous events. The electronic recoils come primarily from $\beta$ decays. Radiogenic neutrons are caused predominantly by spontaneous fission and alpha-neutron reactions from the uranium and thorium chains in the detector components. The CNNS are caused by solar and atmospheric neutrinos, as explained in Section 2.3.3.1. When uncorrelated S1s and S2s are detected, they are labeled as accidental coincidences. Wall leakage events are inward-reconstructed events from near the wall of the TPC. The last type of background, anomalous events, accounts for events with an anomalous S2. This type of background has been observed in XENON100 and in calibration data, however the physical origin is still under investigation. The $\mu$'s and PDF's in Equation 8.1 are determined by multiple input parameters, such as the event rate of the source, the WIMP mass, the WIMP detection efficiency and the uncertainties in the background and signal sources.

The likelihood function must be evaluated at many different WIMP masses during the calculation of the Bayesian upper limit. It would take a lot of process time when the PDFs in the likelihood function were evaluated at all those masses. Therefore, the PDFs are pre-computed at several WIMP masses, called anchor points. When the likelihood function is called at a specific mass, the PDFs will be interpolated between these anchor PDFs. Similarly, the expected number of events is also interpolated between the anchor points. This interpolation results in Bayesian upper limits that are not perfectly smooth. The upper limits could be made smooth artificially, however this is not considered in this work.

In addition to the WIMP mass, the cross section, and the nuisance parameters, the likelihood function in Equation 8.1 also depends on the assumed values of poorly known astrophysical parameters. In most direct detection experiments these parameters are kept fixed by taking the mean values that are preferred by the Standard Halo Model (SHM). The SHM assumes a Maxwellian distribution for the WIMP velocities, with fixed values for the orbital velocity of the Sun, the escape velocity of dark matter from the halo, and the local dark matter density [46]. These values are given in Table 8.1.

<table>
<thead>
<tr>
<th>Observable</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orbital velocity of the Earth</td>
<td>$v_{\text{Earth}}$</td>
<td>232 km s$^{-1}$</td>
</tr>
<tr>
<td>Escape velocity of dark matter</td>
<td>$v_{\text{esc}}$</td>
<td>544 km s$^{-1}$</td>
</tr>
<tr>
<td>Local dark matter density</td>
<td>$\rho_{\odot}$</td>
<td>0.3 GeV cm$^{-3}$</td>
</tr>
<tr>
<td>Solar circular velocity</td>
<td>$v_0$</td>
<td>220 km s$^{-1}$</td>
</tr>
</tbody>
</table>

Table 8.1: Assumed Standard Halo Model parameters used in the likelihood function [46].
8.2 XENON1T’s frequentist upper limit

After applying the selection criteria, the first science run of XENON1T contains a total of 63 events in the 34.2-day dark matter search data. Figure 8.1 presents the 90% CL frequentist upper limit on the WIMP-nucleon cross section of this first science run. All the upper limits in the figure that are shown as reference are also calculated with frequentist statistics. The XENON1T collaboration currently has the most stringent upper limits on the WIMP-nucleon cross section for WIMP masses above 10 GeV/c^2.

Figure 8.1: The WIMP-nucleon cross section frequentist upper limits as a function of WIMP mass at 90% CL (black) for the first science run of XENON1T [45]. The 1σ and 2σ sensitivity bands are denoted by the green and yellow bands, respectively. The upper limits from LUX [26] (red), PandaX-II [47], and XENON100 [24] (gray) are shown for reference.

As Figure 8.1 shows, the upper limits from the various direct dark matter experiments display a typical curved shape. This is caused by two different phenomena. At low WIMP masses, the sensitivity of the experiment drops due to the effective energy threshold of the detector. At high masses the sensitivity decreases as well, because for a fixed mass density, the flux of WIMPs decreases proportionally to 1/m_χ. The best sensitivity is found at WIMP masses that are near the mass of the recoiling xenon nucleus. This published frequentist XENON1T upper limit and its sensitivity bands will be used as a reference for the Bayesian upper limits that are calculated in the following sections.
8.3 XENON1T’s Bayesian upper limit

It is hard to theoretically support a specific region in the \( \{ m_\chi, \sigma \} \)-plane where the WIMPs are expected to exist. Nonetheless, the range where the log-prior in Equation 7.6 is non-zero (and thus the prior belief in what region the detector will detect WIMPs) must be specified. The same approach as [43] is followed, which takes ranges that correspond to the parameter space in which the current best dark matter upper limits are set. Based on Figure 8.1, this results in taking a log-prior for \( m_\chi \) that is uniform in the range \( 5 \times 10^4 \) GeV/c\(^2\) and a uniform log-prior for \( \sigma \) in the range \( 10^{-47} - 10^{-43} \) cm\(^2\).

It is possible to introduce nuisance parameters into Bayesian inference. Each new nuisance parameter then adds an extra dimension to the prior distribution. They are taken care of by integrating them out, which is called marginalization. However, it can be a difficult task to numerically integrate over a multidimensional function. A method such as Markov Chain Monte Carlo could be used to approximate the multidimensional integral, however it is hard to assess the accuracy of such a method. Therefore, nuisance parameters are not considered in the process of setting a Bayesian upper limit. Figure 8.2 shows the XENON1T’s Bayesian upper limit at various confidence levels.

![Figure 8.2: Bayesian upper limits for the first science run of XENON1T. The numbers in the upper limits denote the corresponding confidence level. The 90% CL frequentist upper limit (blue) that has been published by the XENON1T collaboration is shown for reference [45]. In dark blue and light blue are the 1- and 2\( \sigma \) sensitivity bands of the frequentist upper limit, respectively.](image-url)
The strongest 90% CL Bayesian upper limit (thick orange line) is found for 35 GeV/c\(^2\) WIMPs, at 6.3 \(\times 10^{-47}\) cm\(^2\). For WIMP masses above 35 GeV/c\(^2\), the Bayesian upper limit lies inside the 1\(\sigma\) sensitivity band of the frequentist upper limit (blue) that is published by the XENON1T collaboration [45]. Recall however that the Bayesian and the frequentist upper limits should be interpreted in different ways, as explained in Section 7.1 and Section 7.4. This makes it hard to compare the regions that are excluded by each of the two statistical methods.

Because there are only 63 data points in SR0 of which none are clear WIMP candidates, it could be that the upper limits that are established from the posterior distribution are strongly dependent on the choice of the prior range of \(m_\chi\) and \(\sigma\). It is therefore important to do an analysis of the priors.

### 8.4 Analysis of the priors

In the analysis of the priors, which is explained in Section 7.3, the 90% CL Bayesian upper limit from Figure 8.2 (thick orange line) is compared with the 90% CL Bayesian upper limits that are created with other priors. First, it is compared with other log-priors that have different ranges where the prior is non-zero. The prior range for the WIMP mass will be kept between 5 - 10\(^4\) GeV. The minimum prior value for the cross section, \(\sigma_{\text{min}}\) in Equation 7.6, will be lowered to \(10^{-46}\) cm\(^2\) and raised to \(10^{-50}\) cm\(^2\) for the comparison. The maximum prior value for the cross section will also be kept fixed at \(10^{-43}\) cm\(^2\). These settings for the three log-priors that are used in the analysis are summarized in Table 8.2. The result of the comparison is shown in Figure 8.3.

<table>
<thead>
<tr>
<th>Cross section (\sigma)</th>
<th>WIMP mass (m_\chi)</th>
<th>Dash pattern in Figure 8.3 (and Figure 8.5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10^{-46} - 10^{-43}) cm(^2)</td>
<td>5 - 10(^4) GeV/c(^2)</td>
<td>Dashed</td>
</tr>
<tr>
<td>(10^{-47} - 10^{-43}) cm(^2)</td>
<td>5 - 10(^4) GeV/c(^2)</td>
<td>Solid</td>
</tr>
<tr>
<td>(10^{-50} - 10^{-43}) cm(^2)</td>
<td>5 - 10(^4) GeV/c(^2)</td>
<td>Dash-dotted</td>
</tr>
</tbody>
</table>

Table 8.2: Log-priors for the analysis of the priors.

Figure 8.3 shows that the Bayesian upper limit is heavily dependent on the chosen range for the cross section prior. For example, when it is assumed that the cross section has a uniform prior probability in log-space in the range \(10^{-50} - 10^{-43}\) cm\(^2\) (dash-dotted line), instead of the range \(10^{-47} - 10^{-43}\) cm\(^2\) (solid line), the Bayesian upper limit becomes weaker up to approximately 66%. Note that this is also outside the 2\(\sigma\) sensitivity band of the frequentist upper limit of XENON1T.

The heavy dependence of the upper limit on the prior is also shown in Figure 8.4, which displays the Bayesian upper limit for the flat-prior from Equation 7.5 (green) as well as for the log-prior from Equation 7.6 (orange). The same prior ranges are used for the flat-prior and the log-prior. The prior range for the WIMP mass is again between 5 - 10\(^4\) GeV, and the prior range for the cross section is fixed at \(10^{-47} - 10^{-43}\) cm\(^2\).
CHAPTER 8. BAYESIAN UPPER LIMIT FOR XENON1T

Figure 8.3: 90% CL Bayesian upper limits on the WIMP-nucleon cross section for XENON1T’s first science run for three different log-priors. Labelling for the 90% CL frequentist upper limit is as in Figure 8.2.

Figure 8.4: 90% CL Bayesian upper limits for the first science run of XENON1T, using the flat-prior and the log-prior for the cross section. For both the flat-prior and the log-prior, the prior range for the WIMP mass is set between $5 - 10^4$ GeV/c$^2$ and the prior range for the cross section is fixed at $10^{-47} - 10^{-43}$ cm$^2$. 
8.4. ANALYSIS OF THE PRIORS

Figure 8.4 is plotted in logarithmic scale, while the flat-prior assigns an equal prior probability to every cross section in linear space. For the flat-prior, this gives the upper region of the plot a much larger prior probability of containing the true value of the cross section. This results in a much smaller exclusion region for the flat-prior. The log-prior, on the other hand, assigns an equal prior probability to every cross section at each order of magnitude, resulting in an upper limit that excludes a much larger area.

Bayesian inference uses two sources of information: prior information, and information that is obtained from the dataset through the likelihood function. The dataset of the first science run of XENON1T contains 63 datapoints, none of which are clear WIMP candidates. Bayesian theory predicts that when a larger amount of data is incorporated into the analysis, the information from the likelihood function may overwhelm the prior beliefs on the parameters [48]. This is tested by analyzing the development of the Bayesian upper limit when more dark matter search data is added. The dark matter search data is created by simulating 300 days of only electronic recoils (ER) in the XENON1T detector. It is assumed that per 34.2 days exactly 62 ER events occur, which is equal to the expected number of events for ER in the fiducial volume of the XENON1T detector [45]. Figure 8.5 shows the development of the 90% CL upper limit on the WIMP-nucleon cross section for 35 GeV/c\(^2\) WIMPs when more data is added to the analysis. Each of the three upper limits uses a different log-priors, which are described in Table 8.2.

![Figure 8.5: Development over time of the 90% CL upper limit of the WIMP-nucleon cross section for 35 GeV/c\(^2\) WIMPs, using the three different log-priors from Table 8.2. The horizontal axis denotes the amount of days that data is simulated, assuming 62 electronic recoil events per 34.2 days of data.](image)
Figure 8.5 shows that the upper limits of the three different priors do not converge towards each other when more data is added to the analysis. Even after 300 days of simulated data, the 90% CL upper limit value for 35 GeV/c^2 WIMPs still heavily depends on the used prior. Apparently, the ER events in the data do not contain enough information to exclude all the parameter space that has a prior probability of containing WIMPs. This simplified simulation thus indicates that implementing more data into the Bayesian inference does not make the upper limit less dependent on the assumptions in the prior.

8.5 Supersymmetry prior

A range for the two-dimensional prior that can be supported by theory, is the range that corresponds to the parameter space where the supersymmetry (SUSY) models expect WIMPs. SUSY is an addition to the Standard Model of particle physics (SM), which assumes that each particle in the SM has a supersymmetry partner particle. This assumption solves multiple shortcomings of the SM, such as explaining the hierarchy problem and the gauge coupling unification. A more detailed explanation of SUSY is given in [49].

Some SUSY configurations predict that the lightest supersymmetric particle is a stable and electrically neutral particle, and that it interacts weakly with the SM particles. This corresponds exactly to what is expected of WIMPs, as explained in Section 2.2.1. WIMPs from these SUSY configurations have therefore been an important candidate for the dark matter experiments. Figure 8.6 shows the regions in the \( \{m_\chi, \sigma\} \)-plane that are favored by five independent SUSY configurations.

![Figure 8.6: WIMP interaction cross section \( \sigma \) versus WIMP mass \( m_\chi \) from several published results and future reach (dashed) of direct WIMP detection experiments [50]. The solid coloured areas between approximately 100 GeV/c^2 and 1000 GeV/c^2 denote the parameter space where the various supersymmetric configurations favor their dark matter candidate.](image)
Some of the configurations in Figure 8.6, such as the WT Neutralino configuration (red region), have already been excluded by the upper limits from dark matter experiments. Future experiments, such as XENONnT and DARWIN, are expected to be able to rule out even more of the SUSY models. One of the SUSY configurations in Figure 8.6 that is not yet fully excluded by the direct dark matter experiments is the radiatively-driven natural supersymmetry (RNS) configuration (green region). The main difference between the RNS configuration and the other SUSY models is that the other SUSY models predict a Higgs mass much lower than the actual value of 125 GeV. The RNS configuration solves this problem by assuming a mass between 100 - 300 GeV/c$^2$ for the Higgsino (the theoretical supersymmetry partner of the Higgs boson), which is explained in more detail in [51].

The RNS configuration is used to show how Bayesian inference can be used to rule out parameter space of a SUSY configuration. Based on Figure 8.6, the RNS configuration is approximated as a rectangular region between 100 - 250 GeV/c$^2$ for the WIMP mass and $10^{-47} - 10^{-44}$ cm$^2$ for the cross section. A log-prior is applied in this region since this is where the RNS configuration expects WIMPs to exist. Figure 8.7 shows the Bayesian upper limit that is the result of this prior combined with the data from SR0.

Based on the Bayesian upper limit from Figure 8.7, it is ruled out with 90% CL that there exists a 100-250 GeV/c$^2$ WIMP with a cross sections above $10^{-45}$ cm$^2$. Apparently, the rectangular shape approximation of the RNS region that is used as a prior causes the Bayesian and frequentist upper limit to appear identical. It has been tested whether a different approximation results in a less similar Bayesian and frequentist upper limit, which is indeed the case. That the Bayesian upper limit and the frequentist upper limit appear similar, is therefore a coincidence.

Figure 8.7: 90% CL Bayesian upper limit for the first science run of XENON1T, using a uniform log-prior between 100 - 250 GeV/c$^2$ for the WIMP mass and $10^{-47} - 10^{-44}$ cm$^2$ for the cross section. Labelling for the 90% CL frequentist upper limit is as in Figure 8.2.
8.6 Credible region with simulated WIMPs

It is interesting to examine what the credible region would look like if there were actual WIMP signals in the first science run data. To do this, WIMPs with a mass of 20 GeV/c^2 are simulated and added to the 63 events in the SR0 dataset. It is assumed that the WIMPs have a WIMP-nucleon cross section of $1.4 \times 10^{-45}$ cm^2, which corresponds to a nominal expected number of 10 WIMP events in the 34.2 live days of search data of SR0. The log-prior is applied, with a range for the WIMP mass between $5 - 10^4$ GeV/c^2 and for the cross section between $10^{-47} - 10^{-43}$ cm^2. The posterior distribution and the corresponding credible intervals for this simulation are shown in Figure 8.8.

With the credible intervals in Figure 8.8, it is possible to infer something about the true WIMP mass and cross section (of this simulation). For example, the 90% CL credible region indicates that there is a 90% probability that the true value of $m_\chi$ and $\sigma$ lies inside that credible region. The smaller the credible region, the smaller the probability that it contains the true WIMP mass and cross section. This valuable information derived from Bayesian inference cannot be obtained with a frequentist confidence region.

![Figure 8.8: Posterior distribution in the \{m,\sigma\}-plane for 10 WIMPs that are simulated on top of the first science run data. It is assumed that the WIMPs have a mass of 20 GeV/c^2 and a WIMP-nucleon cross section of $1.4 \times 10^{-45}$ cm^2, which is indicated by the yellow cross. Each orange line encloses a credible region, where the corresponding number indicates the CL. The gray colour scale denotes the posterior PDF values, where a lower (higher) posterior PDF corresponds to a lighter (darker) background. The posterior PDF is normalized with respect to the maximum PDF value.](image-url)
Chapter 9

Conclusion and Discussion

Despite the large amount of indirect evidence for dark matter from various cosmological observations, clear evidence for the existence of a dark matter particle explaining these observations remains absent. Dark matter direct detection experiments try to provide this evidence by detecting the interactions between ordinary matter and WIMPs, which are hypothetical particles that are thought to constitute dark matter. One of these experiments is the XENON1T experiment, which currently has the lowest background ever achieved in a dark matter detector. In this thesis, we have described the research conducted in the context of this experiment: the detection principle of the XENON1T detector (Chapter 3), the processor Pax and its subsystems that analyze the data (Chapter 4), the optimization of the thresholds to detect potential WIMP signals in the data (Chapters 5 and 6), and finally Bayesian inference as an alternative statistical framework to set upper limits on the WIMP-nucleon cross section (Chapters 7 and 8).

In the analysis of the hitfinder in Chapter 5, the height of the upper threshold was optimized. The hitfinder algorithm determines whether there are hits inside a pulse. With an optimized upper threshold, the hitfinder is able to find as many one- or multiple photoelectron signals in the data as possible, while it triggers as few as possible when there are no photons. For the first science run (SR0) analysis of XENON1T, a hitfinder upper threshold between 3 and 6 times the average noise level of a pulse was found to be optimal. In future research, improvements can be made by determining the threshold for each PMT individually. The overall effect of such an analysis may however be small since the upper threshold is already dynamic as it depends on the noise level of each pulse.

In Chapter 6 an improved hitfinder algorithm was introduced and optimized, such that long-tailed pulses get fully integrated. The new algorithm causes the domain over which the pulse is integrated to be defined by a fixed amount of time before and after the hit passes the upper threshold. It was found that the
optimal integration of a pulse starts 10 ns before it passes the upper threshold, and stops 200 ns after it passes the upper threshold. These settings were subsequently implemented into the analysis of SR0.

After determining the optimal settings for the thresholds for the hitfinder algorithm, Bayesian inference was performed to set an upper limit on the WIMP-nucleon cross section using the SR0 data of XENON1T. Dark matter experiments normally report upper limits that are based on frequentist statistics, however one of the problems with frequentist statistics is that it tends to say more about the probability of observing a similar upper limit in future dark matter experiments with the same expected signal and background, than about the non-existence of the signal itself. Furthermore, frequentist statistics does not allow implementing prior knowledge regarding the WIMP mass and the WIMP-nucleon cross section. By using Bayesian inference, an upper limit on the cross section was obtained which appears to improve upon XENON1T’s published frequentist limit, for all WIMP masses. The strongest upper limit is found for 35 GeV/c$^2$ WIMPs, at $6.3 \times 10^{-47}$ cm$^2$. However, due to different interpretations of the Bayesian and the frequentist upper limit, it is not possible to draw conclusions from comparing the two limits. A disadvantage of using Bayesian inference is that any choice for a specific prior is in fact an arbitrary choice. The XENON1T’s Bayesian upper limit turned out to be highly sensitive to these prior beliefs on the true WIMP mass and the WIMP-nucleon cross section. This sensitive dependence of the upper limit on the non-objective choice for a specific prior makes Bayesian inference an unsuitable method for setting the upper limit for the XENON1T experiment.

It would be interesting to repeat the Bayesian analysis in the future with an alternative prior probability density function. For example, the upper limits from previous experiments could be taken as a basis for the prior belief on the parameters, instead of the uniform distribution. Incorporating nuisance parameters into the analysis, such as the uncertainties in the background and signal sources, could also extend the Bayesian inference. When successfully implemented, this should make the XENON1T Bayesian upper limit more robust against the uncertainties that the nuisance parameters represent.
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During the past year, I have gained an enormous amount of knowledge in dark matter and how dark matter data at a large experiment like XENON1T is analyzed. I was fortunate enough to control the detector for more than two weeks in Gran Sasso, as well as witnessing the process of publishing XENON1T’s first dark matter results. Among other things, these two experiences have taught me a lot about performing scientific research.

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Bibliography


