

Goodness-of-Fit Testing using Wasserstein Distance to evaluate model of Double Electron Capture background

Nevis Labs Columbia University REU
XENON Collaboration

Eleni Mandarakas

eleni.mandarakas@gmail.com

Bucknell University



XENON

Mentors: Prof. Elena Aprile
Dr. Pueh Leng Tan

Introduction to XENON

Dark Matter and Other Exotic Particles

Introduction to
XENON

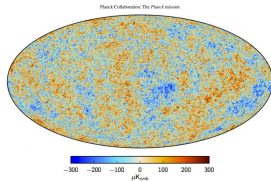
Double Electron
Capture (DEC)

Hypothesis
Testing

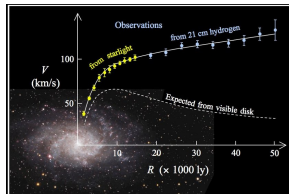
Wasserstein
Distance

Methodology

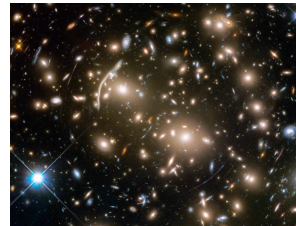
Conclusion



Temperature
Fluctuations in CMB
[7]



Rotation Curves of
Speeds of Galaxies [9]



Gravitational Lensing
[10]

Introduction to
XENON

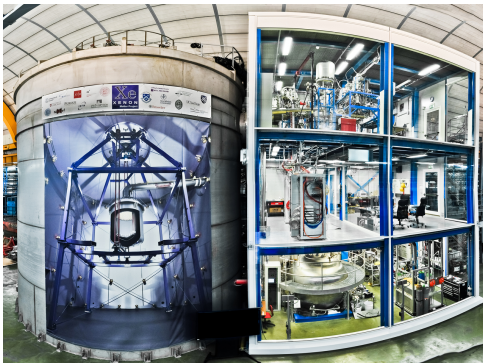
Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

Methodology

Conclusion



XENON Detector [4]



Laboratori Nazionali del Gran Sasso
(LNGS) [8]

Dual Phase Xenon Time Projection Chamber (TPC)

Introduction to
XENON

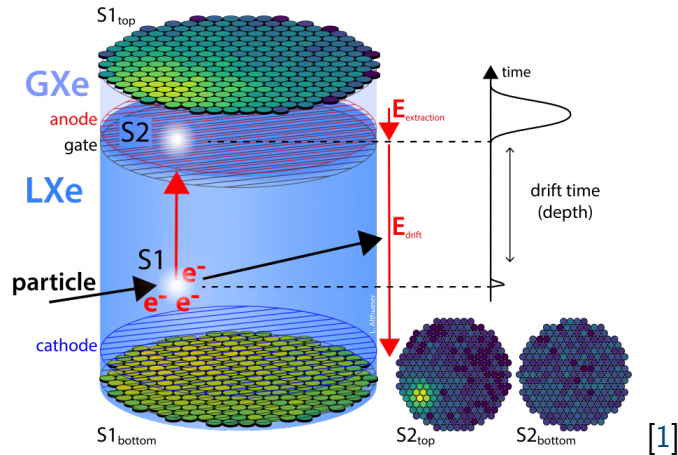
Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

Methodology

Conclusion



ER and NR Discrimination

Introduction to
XENON

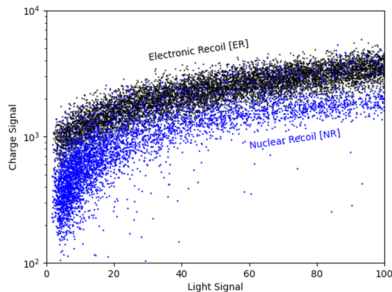
Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

Methodology

Conclusion



[12]
NR:

- ◇ Nuclear Recoil
- ◇ Particle collides with nucleus / Xe atom
- ◇ ROI to find WIMPs
- ◇ high ionization density $\rightarrow$ high recombination rate $\rightarrow$ lower charge yield

ER:

- ◇ Electronic Recoil
- ◇ Particle collides with electron
- ◇ Background
- ◇ low ionization density $\rightarrow$ low recombination rate $\rightarrow$ higher charge yield

Double Electron Capture (DEC)

Double Electron Capture (DEC)



Introduction to
XENON

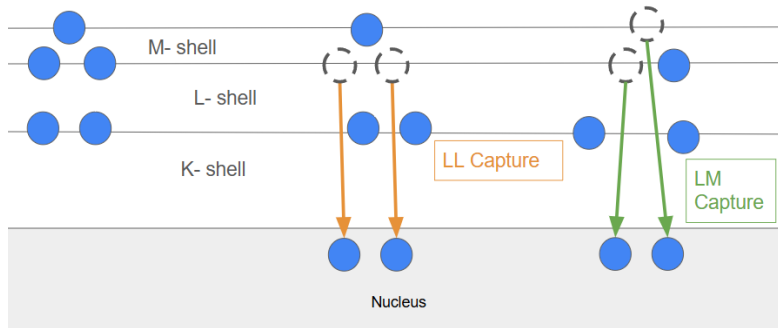
Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

Methodology

Conclusion



Double Electron Capture (DEC)



Introduction to
XENON

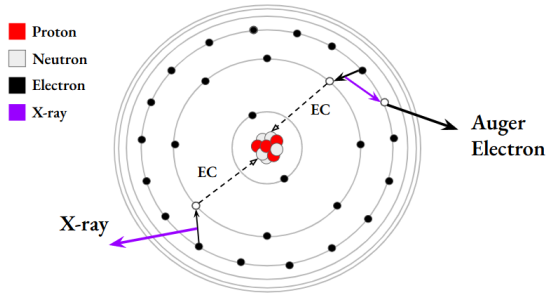
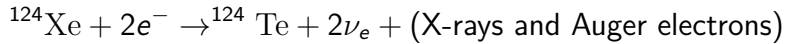
Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

Methodology

Conclusion



Double Electron Capture (DEC)



Introduction to
XENON

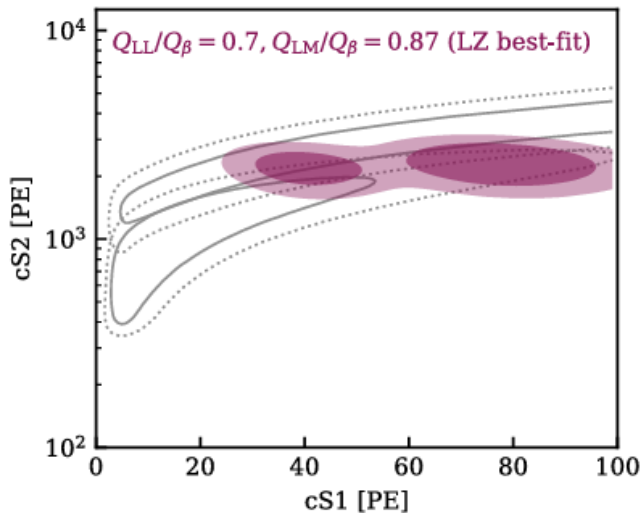
Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

Methodology

Conclusion



[6]

Hypothesis Testing

Hypothesis Testing

Goodness of Fit Test - One Tail

Goodness of Fit Test

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

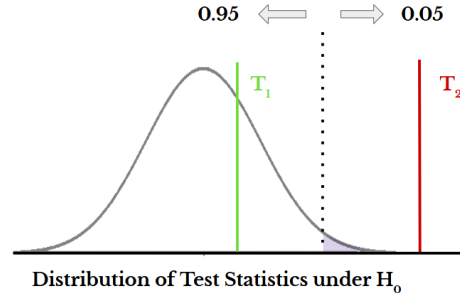
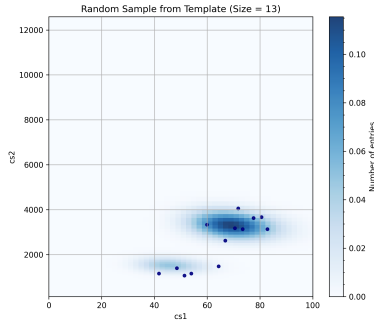
Goodness of Fit Test
- One Tail
Power

Wasserstein
Distance

Methodology

Conclusion

- ◇ Calculate the test statistic - the difference between data and model.
- ◇ Compare statistic to test distribution under H_0 to see if it falls beyond the defined confidence interval (e.g. 95%).
- ◇ If beyond, reject the null.



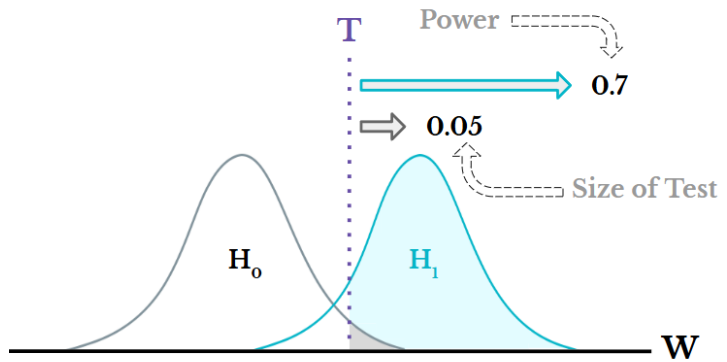
Hypothesis Testing

Power

Power Calculation

- Introduction to XENON
- Double Electron Capture (DEC)
- Hypothesis Testing
- Goodness of Fit Test - One Tail
- Power
- Wasserstein Distance
- Methodology
- Conclusion

$$\text{Power} = P_{H_1}(W > T)$$



Wasserstein Distance

Wasserstein Distance

General Definition

General Definition: Wasserstein Distance

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

General Definition
EMD Function
Wasserstein
Distribution

Methodology

Conclusion

The Wasserstein distance, also known as the Earth Mover's Distance (EMD), measures the minimum "work" required to transform one probability distribution into another, where "work" = (amount of mass moved) $\times$ (distance transported).

Formal Definition:

$$W_p(\mu, \nu) = \left(\inf_{\gamma \in \Gamma(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^p d\gamma(x, y) \right)^{1/p}$$

Where:

- ◇ μ, ν : input distributions
- ◇ $\gamma \in \Gamma(\mu, \nu)$: set of all joint couplings with marginals μ, ν
- ◇ $d(x, y)$: metric distance between points x and y

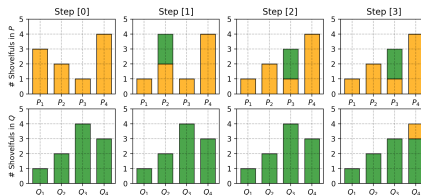


Figure 1. Discrete 1D example of EMD [11].

Wasserstein Distance

EMD Function

2-Wasserstein Distance (EMD) Formulation

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

General Definition
EMD Function
Wasserstein
Distribution

Methodology

Conclusion

Source: $\{x_i\}_{i=1}^n \subset \mathbb{R}^2, \mathbf{a} \in \mathbb{R}^n$

Target: $\{y_j\}_{j=1}^m \subset \mathbb{R}^2, \mathbf{b} \in \mathbb{R}^m$

$$\sum_{i=1}^n a_i = 1, \quad \sum_{j=1}^m b_j = 1, \quad a_i, b_j \geq 0$$

Cost matrix: $C_{ij} = \|x_i - y_j\|_2^2$

Transport plan: $\gamma \in \mathbb{R}^{n \times m}$

$$\begin{aligned} \sum_{j=1}^m \gamma_{ij} &= a_i \quad \forall i & \gamma_{ij} &\geq 0 \quad \forall i, j \\ \sum_{i=1}^n \gamma_{ij} &= b_j \quad \forall j \end{aligned}$$

2-Wasserstein Distance:

$$W = \left(\sum_{i=1}^n \sum_{j=1}^m \gamma_{ij} C_{ij} \right)^{1/2}$$

Source Distribution

Event Locations: $x = \left\{ \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \begin{pmatrix} 3 \\ 4 \end{pmatrix}, \begin{pmatrix} 3 \\ 4 \end{pmatrix} \right\}$

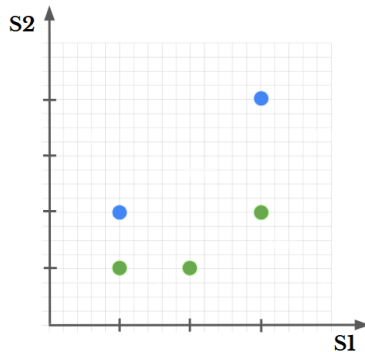
Locations: $x = \{(1, 2), (3, 4)\}$

Masses: $\mathbf{a} = [0.5, 0.5]$

Target Distribution

Locations: $y = \{(2, 1), (3, 2), (1, 1)\}$

Masses: $\mathbf{b} = [0.25, 0.5, 0.25]$



Numerical Example: Cost Matrix $C_{ij} = \|x_i - y_j\|_2^2$

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

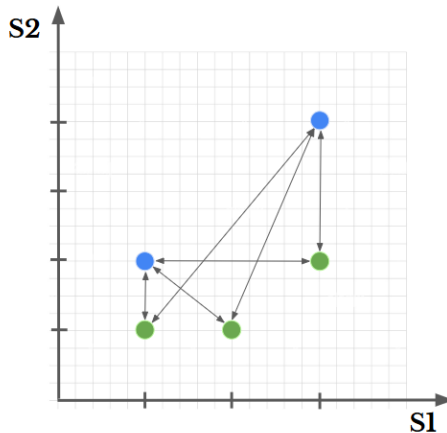
General Definition
EMD Function
Wasserstein
Distribution

Methodology

Conclusion

	$y_1 = (2, 1)$	$y_2 = (3, 2)$	$y_3 = (1, 1)$
$x_1 = (1, 2)$	2	4	1
$x_2 = (3, 4)$	10	4	13

$$C = \begin{bmatrix} 2 & 4 & 1 \\ 10 & 4 & 13 \end{bmatrix}$$



Mass Marginals and Optimal Transport Plan

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

General Definition
EMD Function
Wasserstein
Distribution

Methodology

Conclusion

Mass marginals:

$$\mathbf{a} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 0.25 \\ 0.5 \\ 0.25 \end{bmatrix}$$

$$\sum_{i=1}^n a_i = 1, \quad \sum_{j=1}^m b_j = 1, \quad a_i, b_j \geq 0$$

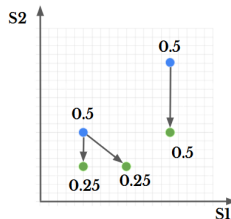
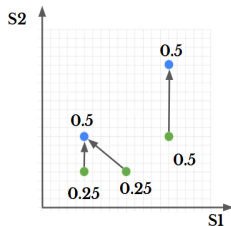
Optimal transport plan:

$$\gamma = \begin{bmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} \\ \gamma_{21} & \gamma_{22} & \gamma_{23} \end{bmatrix}$$

$$\sum_{j=1}^3 \gamma_{ij} = a_i \quad (\text{row sums})$$

$$\sum_{i=1}^2 \gamma_{ij} = b_j \quad (\text{column sums})$$

$$\gamma_{ij} \geq 0 \quad (\text{non-negativity})$$



Solution: $\gamma = \begin{bmatrix} 0.25 & 0 & 0.25 \\ 0 & 0.5 & 0 \end{bmatrix}$

$$C = \begin{bmatrix} 2 & 4 & 1 \\ 10 & 4 & 13 \end{bmatrix}, \quad \gamma = \begin{bmatrix} 0.25 & 0 & 0.25 \\ 0 & 0.5 & 0 \end{bmatrix}$$

Compute total cost:

$$\sum_{i=1}^2 \sum_{j=1}^2 \gamma_{ij} C_{ij} = 0.25 \cdot 2 + 0.25 \cdot 1 + 0.5 \cdot 4 = 2.75$$

2-Wasserstein Distance:

$$W = \left(\sum_{i,j} \gamma_{ij} C_{ij} \right)^{1/2} = \sqrt{2.75} \approx 1.66$$

Wasserstein Distance

Wasserstein Distribution

Visualizing a Wasserstein Distribution

Introduction to
XENON

Double Electron
Capture (DEC)

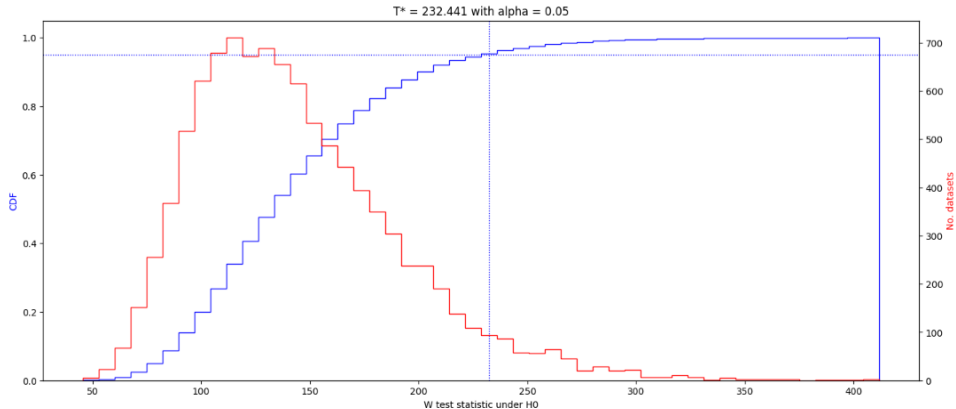
Hypothesis
Testing

Wasserstein
Distance

General Definition
EMD Function
Wasserstein
Distribution

Methodology

Conclusion



Distribution Free? - Varying Mean



Introduction to
XENON

Double Electron
Capture (DEC)

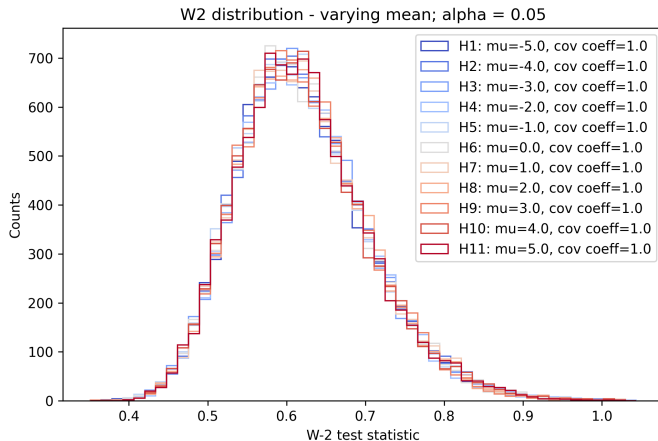
Hypothesis
Testing

Wasserstein
Distance

General Definition
EMD Function
Wasserstein
Distribution

Methodology

Conclusion



Distribution Free? - Varying Covariance



Introduction to
XENON

Double Electron
Capture (DEC)

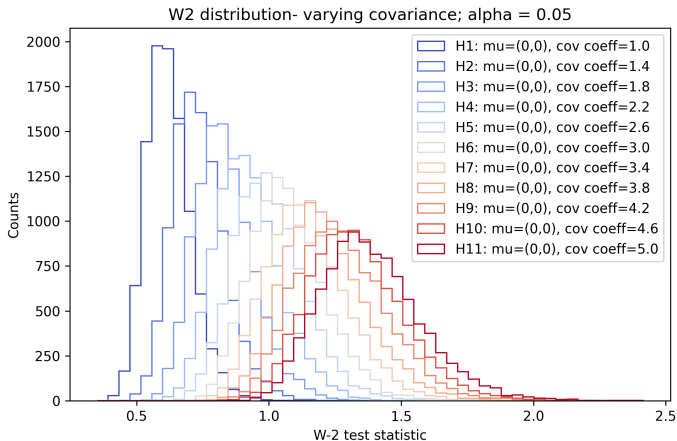
Hypothesis
Testing

Wasserstein
Distance

General Definition
EMD Function
Wasserstein
Distribution

Methodology

Conclusion



Conclusion

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

Wasserstein
Distance

General Definition
EMD Function
Wasserstein
Distribution

Methodology

Conclusion

- ◇ Not Distribution Free
- ◇ Monte Carlo Random Sampling to approximate distribution for each H_0

Methodology

Methodology

Templates

Template

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

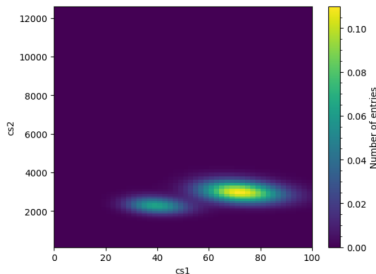
Wasserstein
Distance

Methodology

Templates
Sampling

Conclusion

- ◇ 2D histogram
- ◇ vary LL and LM parameter by changing the light and charge yield
- ◇ 11 variations of LL Parameter/11 variations of LM Parameter - 121 possible templates



Vary LL and LM Parameter Individually

Introduction to
XENON

Double Electron
Capture (DEC)

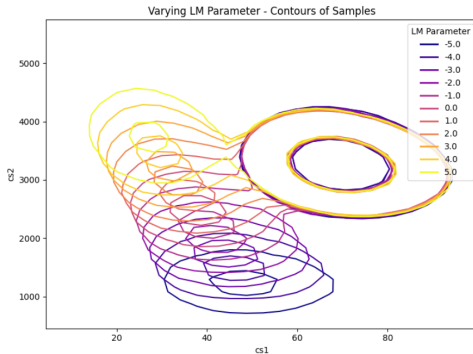
Hypothesis
Testing

Wasserstein
Distance

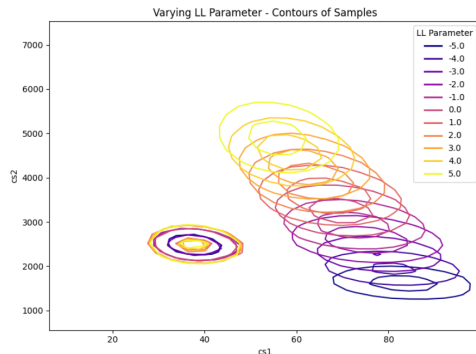
Methodology

Templates
Sampling

Conclusion



Varying LM Parameter - LL Parameter
fixed at 0.0



Varying LL Parameter - LM Parameter
fixed at 0.0

Methodology

Sampling

Samples

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

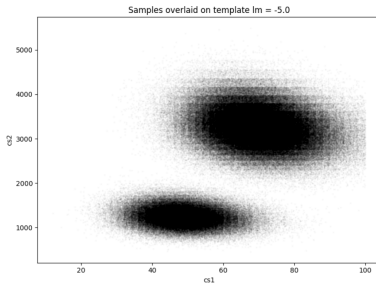
Wasserstein
Distance

Methodology

Templates
Sampling

Conclusion

- ◇ Sample size = 13 $\rightarrow$ expect to see approximately 13 DEC Events in the data set
- ◇ Template - use bin centers and "height" of bin to construct probability distribution
- ◇ Redraw sample and compare with template 10,000 times to create Wasserstein Distribution



Conclusion

Conclusion

Results

Power Heatmap



Introduction to
XENON

Double Electron
Capture (DEC)

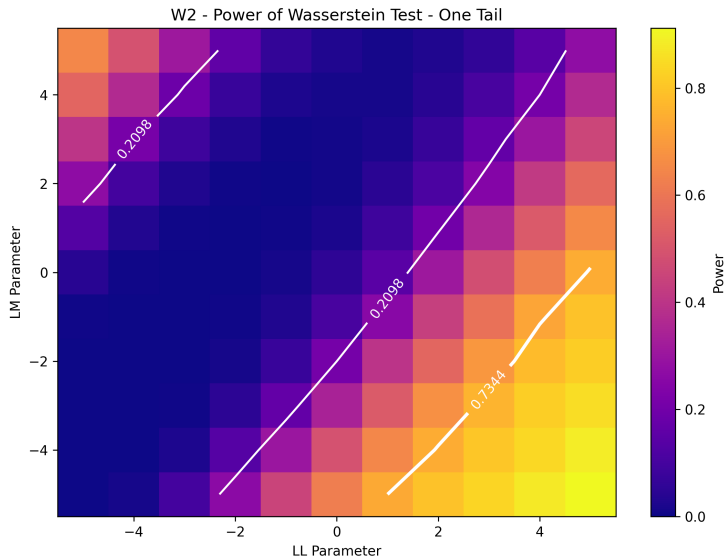
Hypothesis
Testing

Wasserstein
Distance

Methodology

Conclusion

Results
Future Work



χ^2 Test Comparison



Introduction to
XENON

Double Electron
Capture (DEC)

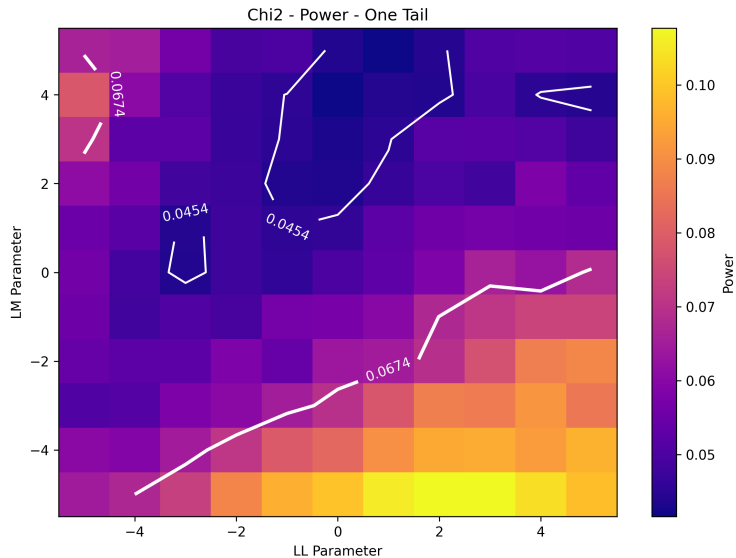
Hypothesis
Testing

Wasserstein
Distance

Methodology

Conclusion

Results
Future Work



Conclusion

Future Work

Two-Tail Power

Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

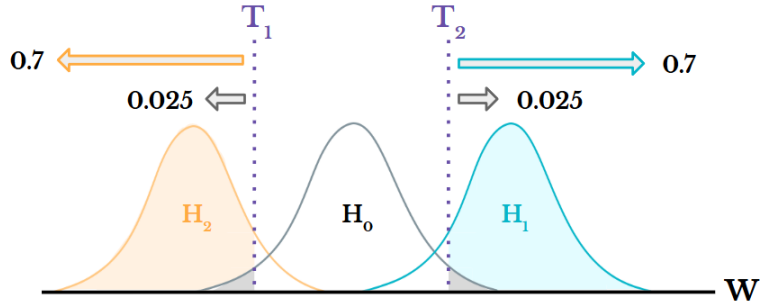
Wasserstein
Distance

Methodology

Conclusion

Results

Future Work



Two-Tail Power Heatmap



Introduction to
XENON

Double Electron
Capture (DEC)

Hypothesis
Testing

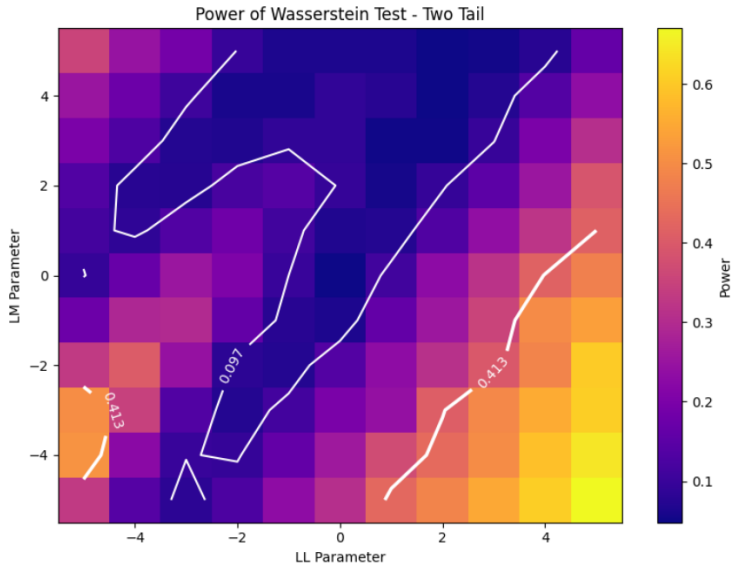
Wasserstein
Distance

Methodology

Conclusion

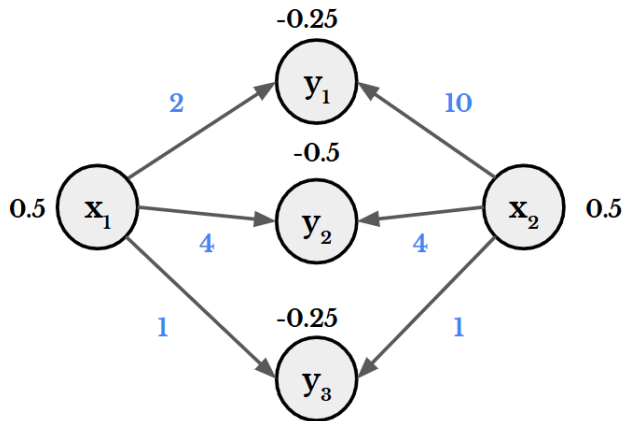
Results

Future Work

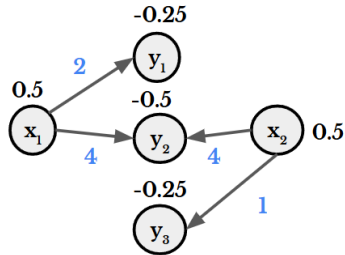


Thank you!

I am grateful to Dr. Elena Aprile for her constant support, Dr. Pueh Leng Tan for her mentorship, direction, and impactful discussions, and XENON Collaboration and Laboratori Nazionali del Gran Sasso for hosting and supporting the project. Thank you also to the Nevis Labs REU Program; Prof. Georgia Karagiori, Prof. Reshmi Mukherjee, Amy Garwood, Asia Latt, and Ashley L. Delphia. This material is based upon work supported by the National Science Foundation under Grant No. PHY-2349438.



Choose Basis:



Cost - Dual Tail + Dual Head = 0

$$2 - 0 - 2 = 0$$

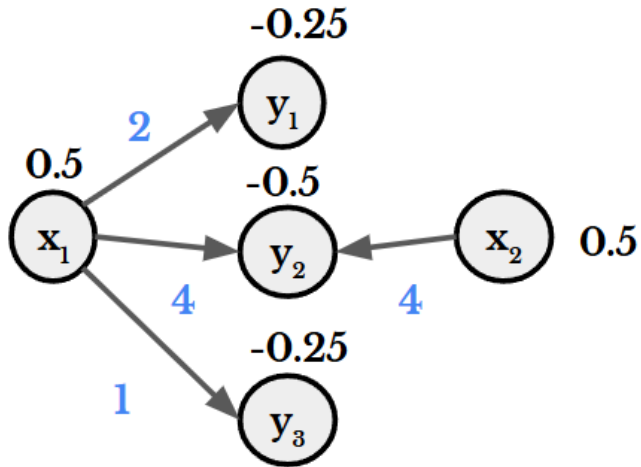
$$4 - 0 - 4 = 0$$

$$4 - 0 - 4 = 0$$

$$1 - 0 - 1 = 0$$

$$x_0 y_1: 10 - 0 - 2 = 8$$

$$x_1 y_3: 1 - 0 - 4 = -3$$





Lutz Althüser.

Schematic of the xenonnt liquid-xenon detector.

Image from XENON Collaboration, credited to Lutz Althüser, n.d.

Retrieved 2025-08-01.



E. Aprile et al.

Observation of two-neutrino double electron capture in ^{124}Xe with xenon1t.

Nature, 568(7753):532–535, 2019.



E. Aprile and XENON Collaboration.

Wimp dark matter search using a 3.1 tonne $\times$ year exposure of the xenonnt experiment.

arXiv preprint, 2025.



ETAP – Experimental Particle and Astroparticle Physics Group, Johannes Gutenberg University Mainz.

Xenon/darwin – ex-xenon research group overview.

<https://www.etap.physik.uni-mainz.de/research-groups/ex-xenon/>, n.d.

Accessed: 2025-08-01.



Marc Hallin, Gilles Mordant, and Johan Segers.

Multivariate goodness-of-fit tests based on wasserstein distance, 2020.



Robert Hammann.

Dec hypothesis test and wimp roi in xenonnt, 2024.

XENON1T Internal Note, accessible via XENON Wiki.



Daniel R. Herrera, U. São Paulo, and S.E. Jorás.

Full-sky map of the cmb temperature anisotropies observed by planck satellite.

<https://www.researchgate.net/figure/>

[Full-sky-map-of-the-CMB-temperature-anisotropies-observed-by-Planck-satellite-Figure_fig1_334447860](#), 2019.

Accessed: 2025-08-01.



Laboratori Nazionali del Gran Sasso.

Lngs overview.

<https://www.lngs.infn.it/en/lngs-overview>, n.d.

Accessed: 2025-08-01.



P.A. Murad.



László Szabados.

Symmetries in stellar, galactic and extragalactic astronomy.

In *Complex Symmetries*, pages 191–206. 2022.



Lilian Weng.

Gan by example (part 1), 2017.

Accessed: 2025-07-22.



XENON Collaboration.

Time projection chamber.

<https://xenonexperiment.org/time-projection-chamber/>, n.d.

Accessed: 2025-08-01.