LAMARR

INSTITUTE FOR
MACHINE LEARNING
AND ARTIFICIAL
INTELLIGENCE

In Machine Learning, *Unfolding* Is Known As *Quantification Learning*

Bridging the Gap: Unfolding & Quantification Learning for Physics Research

Mirko Bunse

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Partner institutions:

technische universität dortmund

Fraunhofer IAIS

UNIVERSITÄT BONN

Fraunhofer IML

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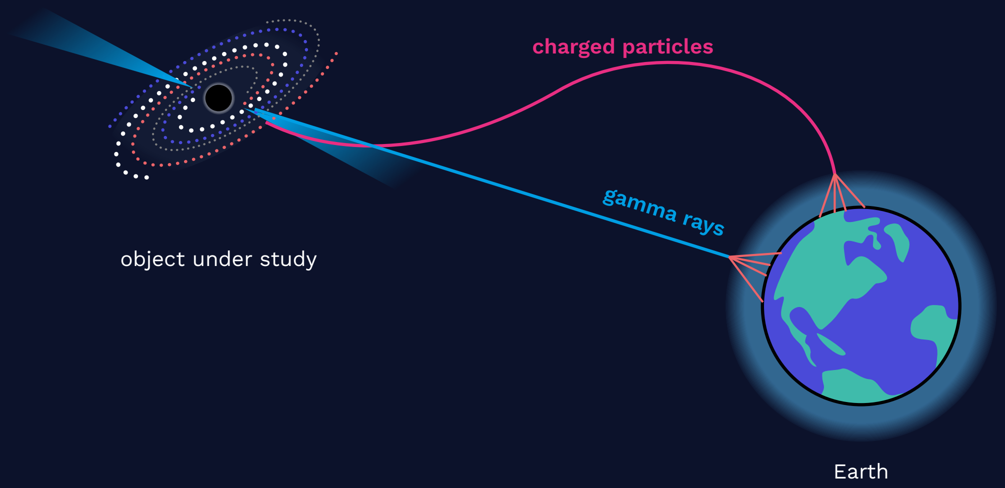
Why Bother?

Research on quantification learning offers:

- Fast-paced improvements of methods
- Few limitations (e.g., no limitation on the number of observables)
- Comprehensive theoretical understanding
- Interdisciplinary community eager to explore new aspects
- Funding opportunities

Example Use Case: Ground-Based Gamma-Ray Observatories



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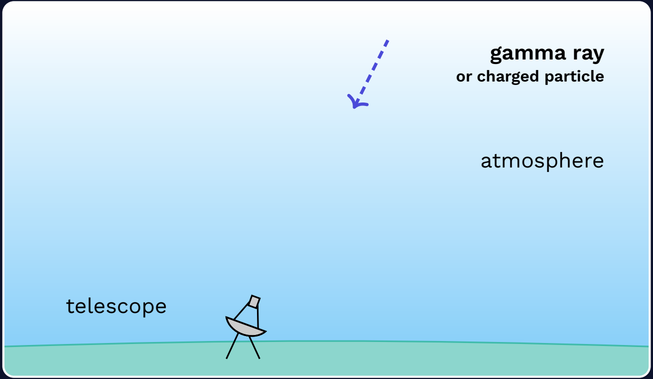

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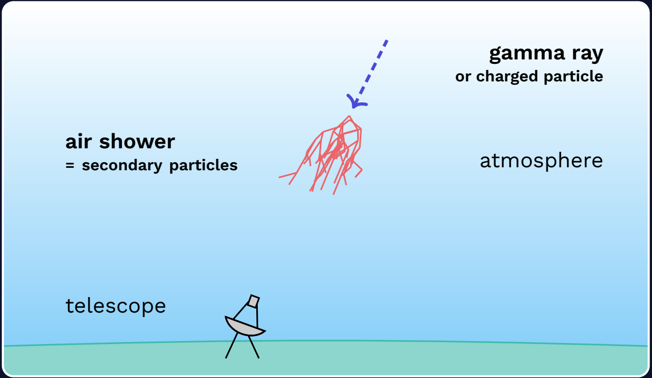

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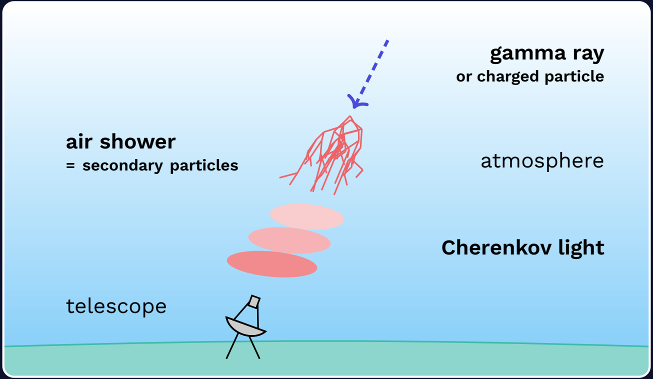

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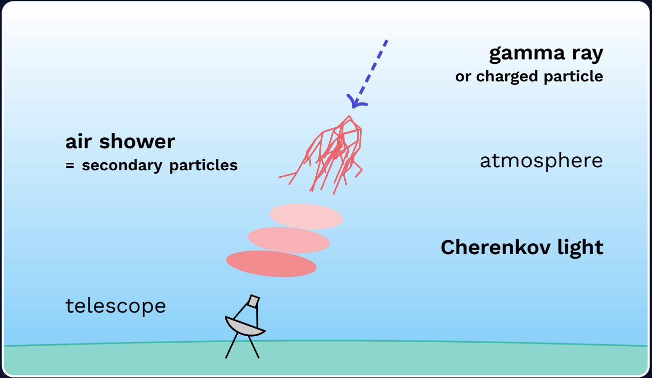

Preprocessing → Background rejection

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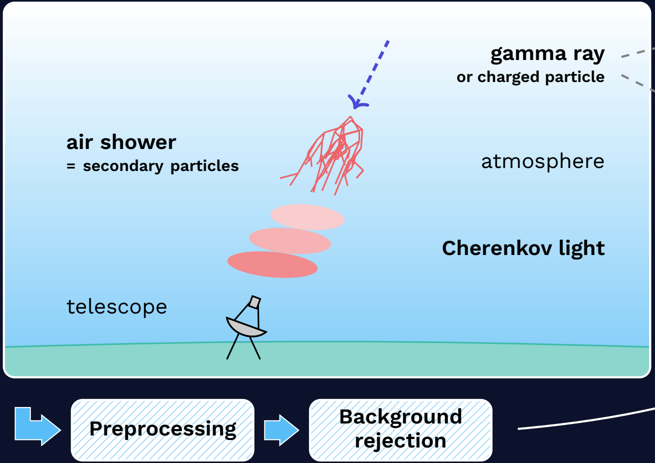

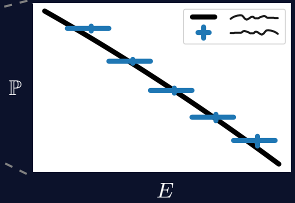

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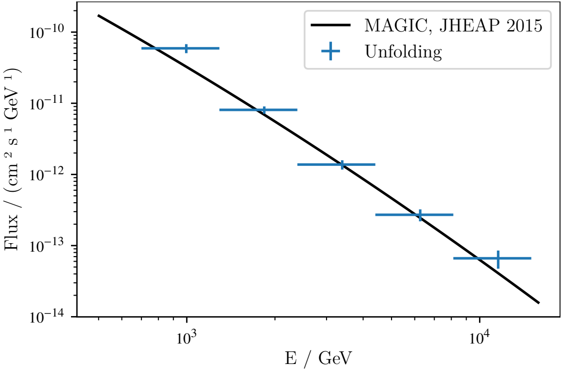
Unfolding: the Reconstruction of Spectra

Goal: reconstruct the spectrum $p(y)$ of some quantity y from a measurement $q(x)$.

$$\underbrace{q(x)}_{\text{measurement}} = \int \underbrace{M(x \mid y)}_{\text{transfer}} \cdot \underbrace{p(y)}_{\text{target}} \, \mathrm{d}y$$



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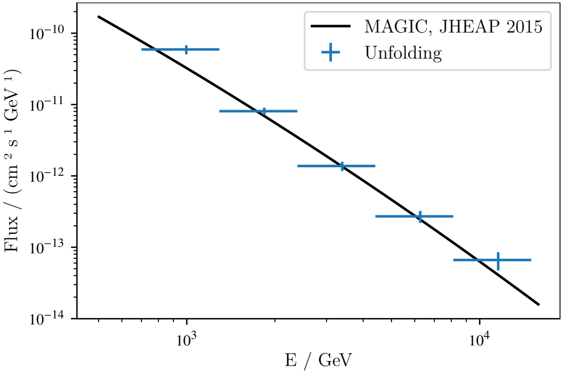
Approach: set up a linear system of equations

$$\mathbf{q} = \mathbf{M}\mathbf{p} \qquad \text{where} \quad \begin{cases} \mathbf{q} = \frac{1}{|\mathrm{B}\,|} \sum_{x \in \mathrm{B}} \phi(x) \\ \mathbf{M}_i = \frac{1}{|\mathrm{D}_i|} \sum_{x \in \mathrm{D}_i} \phi(x) \end{cases}$$



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and solve it by minimizing some loss, i.e.,

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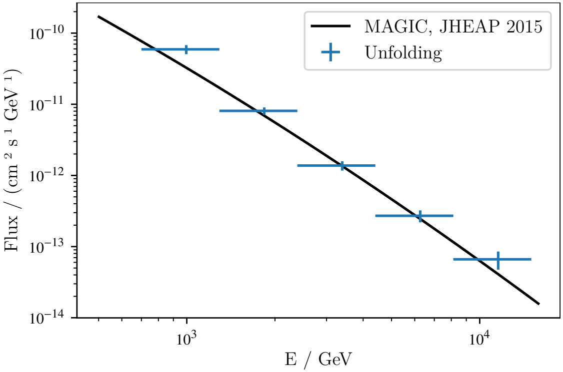

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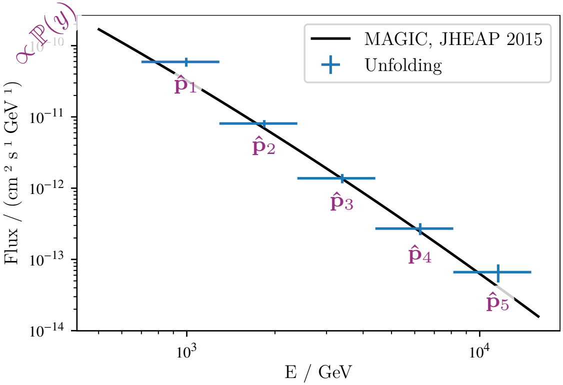

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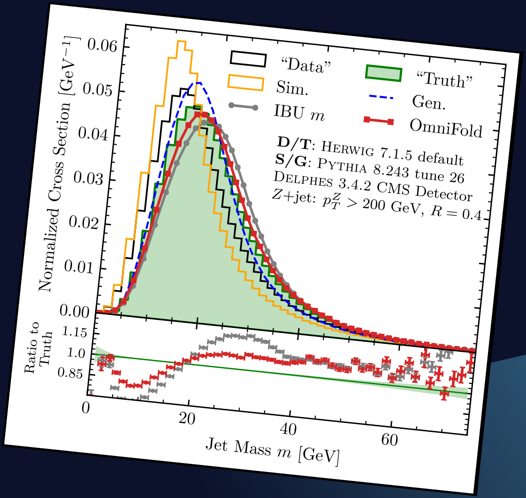
Use Cases Everywhere: Count + Predict



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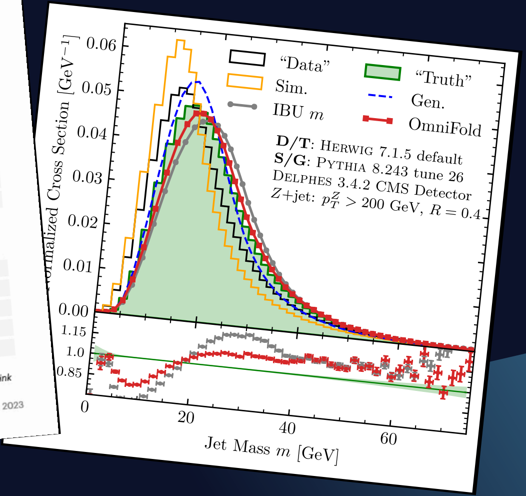

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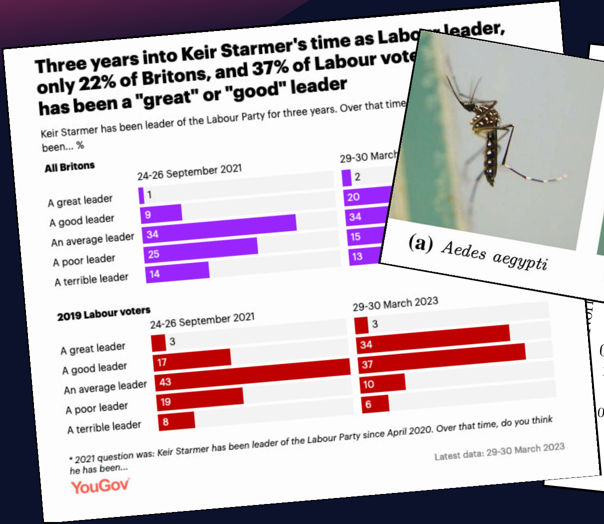
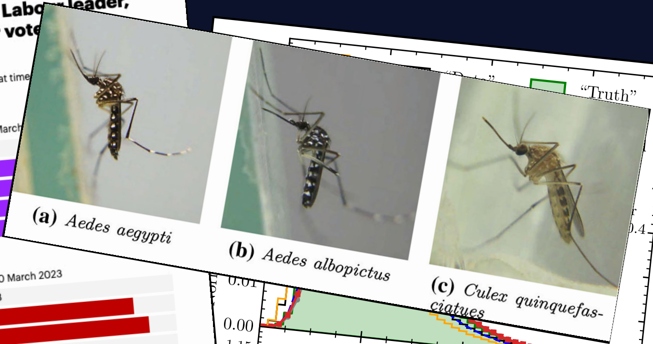
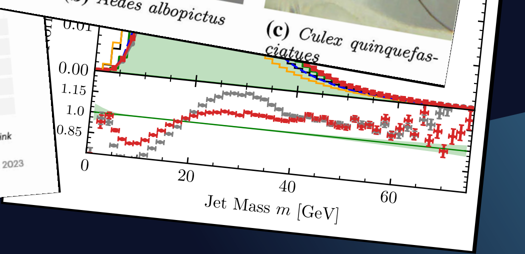



(a) *Aedes aegypti* (b) *Aedes albopictus* (c) *Culex quinquefasciatus*



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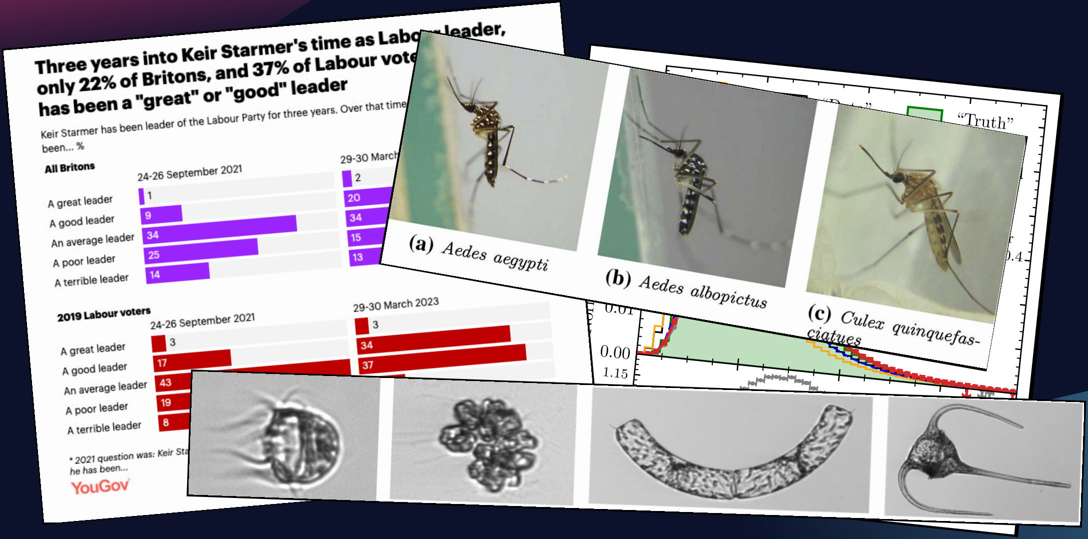

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In Computer Science, unfolding-like problems are covered by **Quantification Learning**[3,4].

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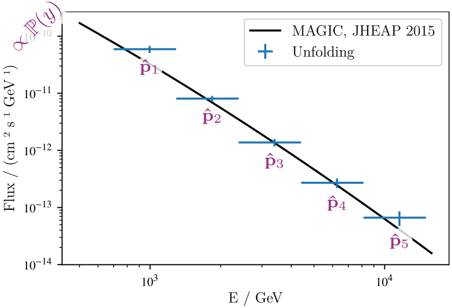

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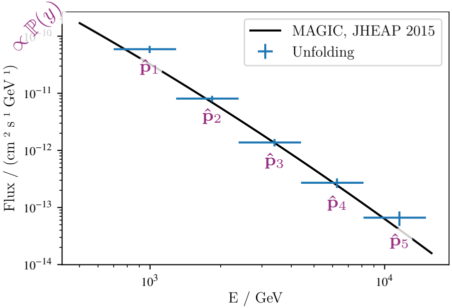
Approach: solve $\mathbf{q} = \mathbf{M}\mathbf{p}$ for $\mathbf{p}$ (just like before!)

Hence, unfolding $\equiv$ quantification.



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5 Learnings From Quantification Research

1st Learning: Statistical Consistency

Definition (Fisher Consistency for Prior Probability Shift):

If a consistent quantifier had access to the entire population $\mathbb{Q}(X)$ (i.e., to "unlimited data"), it would return the true class prevalences:

$$\underbrace{h'\big(\mathbb{Q}(X)\big)}_{\substack{\text{population}\\\text{analogue}\\\text{of } h(\mathrm{B})}} = \mathbb{Q}(Y) \quad \underbrace{\forall\ \mathbb{Q} : \mathbb{Q}(X \mid Y) = \mathbb{P}(X \mid Y)}_{\text{for any } \mathbb{Q} \text{ with PPS}}$$

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- not a sufficient but certainly **a necessary criterion** for quantifier selection

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1) RUN[5] **/ TRUEE** (and others) *are* Fisher consistent[6] ✓

2) DSEA & DSEA+ are *not* Fisher consistent[7] ✗

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2nd Learning: The Anatomy of Prediction Errors

Prediction Error Bound:[8] describes the *impact of* and the *interplay between* causes of errors.

$$\underbrace{\left\| h(\mathrm{B}) - \mathbf{p}^* \right\|_2}_{\text{prediction error}} \leq \underbrace{\frac{2k(2 + \sqrt{2 \log \frac{2C}{\delta}})}{\sqrt{\lambda_2}}}_{\text{representation } \phi} \cdot \left(\underbrace{\left\| \frac{\mathbf{p}^*}{\mathbf{p}_{\mathrm{trn}}} \right\|_2}_{\text{shift}} \cdot \underbrace{\frac{1}{\sqrt{|\mathrm{D}|}}}_{\text{volume } \mathrm{D}} + \underbrace{\frac{1}{\sqrt{|\mathrm{B}|}}}_{\text{volume } \mathrm{B}} \right)$$

where

- $h(\mathrm{B})$ is the solution of $\mathbf{q} = \mathbf{M}\mathbf{p}$
- k is a constant s.t. $\|\phi(x)\|_2 \leq k \;\forall\, x \in \mathcal{X}$
- λ_2 is the second-smallest eigenvalue of some particular $\mathbf{G}$
- δ is the desired probability

[8] Dussap, Blanchard, and Chérief-Abdellatif, "Label Shift Quantification with Robustness Guarantees via Distribution Feature Matching", 2023, .

3rd Learning: Improved Optimization Techniques

Algorithm	Estimate	Validity
RUN[5]	$\hat{\mathbf{p}} = \underset{\mathbf{p} \in \mathbb{R}^C}{\arg\min} \; \ell(\mathbf{p};\ \mathbf{q}, \mathbf{M})$	invalid: $\hat{\mathbf{p}} \notin \Delta^{C-1}$ ✗

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Constrained[10]	$\hat{\mathbf{p}} = \underset{\mathbf{p} \in \Delta^{C-1}}{\arg\min} \; \ell(\mathbf{p};\; \mathbf{q}, \mathbf{M})$	valid ✓
Soft-Max[10]	$\hat{\mathbf{p}} = \sigma(\mathbf{l}^*) , \quad \mathbf{l}^* = \underset{\mathbf{l} \in \mathbb{R}^{C-1}}{\arg\min} \; \ell(\sigma(\mathbf{l})\; ; \; \mathbf{q}, \mathbf{M})$	valid ✓

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4^{th} Learning: Methods Are Numerous

Most methods are combinations of

- a data representation $\phi : \mathcal{X} \rightarrow \mathcal{Z}$
- a loss function $\ell : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathbb{R}$
- an optimization algorithm

These components can be recombined to even more methods.

[11] Bella et al., “Quantification via Probability Estimators”, 2010, .

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github.com/mirkobunse/qunfold

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Representations: hard[4] & soft[11] classification, histograms[12], tree-based binnings[13], kernel means[14], ...

Loss Functions: least squares[4,11], Hellinger distance[12], energy distance[14], Poisson likelihood[5], ...

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5th Learning: Open Issues in Quantification Research

Complications of experimental physics:

- ordinality: $y_i \prec y_{i+1} \ \forall \, i \in \mathcal{Y}$ (to be covered through regularization for ordinal plausibility[15])

[15] Bunse et al., "Regularization-based Methods for Ordinal Quantification", 2024.

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- changing environment: $\mathbb{Q}(\mathbf{x}, y) = \sum_{e \in \mathcal{E}} \mathbb{Q}(\mathbf{x}, y, e)$

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- inspect contributions of individual data items $\mathbf{x} \in \mathrm{B}$ to $h(\mathrm{B})$ (data selection, human in the loop)

Hence, there are substantial opportunities for quantification-related research in Computer Science.

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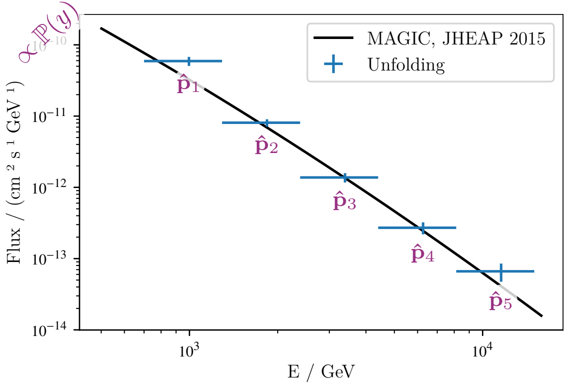
$$\underbrace{q(x)}_{\text{measurement}} = \int \underbrace{M(x \mid y)}_{\text{transfer}} \cdot \underbrace{p(y)}_{\text{target}} \, \mathrm{d}y$$

Approach: set up a linear system of equations

$$\mathbf{q} = \mathbf{M}\mathbf{p} \qquad \text{where} \begin{cases} \mathbf{q} = \frac{1}{|\mathrm{B}\,|} \sum_{x \in \mathrm{B}} \phi(x) \\ \mathbf{M}_i = \frac{1}{|\mathrm{D}_i|} \sum_{x \in \mathrm{D}_i} \phi(x) \end{cases}$$

and solve it by minimizing some loss, i.e.,

$$\hat{\mathbf{p}} = \underset{\mathbf{p} \in \Delta^{C-1}}{\arg\min} \; \ell(\mathbf{p};\; \mathbf{q}, \mathbf{M})$$



unknown $y \in [1, 5]$

$\equiv$ class label!

[2] Fig.: Morik and Rhode, *Machine Learning under Resource Constraints – Discovery in Physics*, 2023

Conclusion: 5 Learnings From Quantification

Understanding of the Problem Statement:

1) Consistency is a necessary criterion for algorithm selection

2) The prediction error is governed by the representation, the amount of shift, and the data volumes

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Improvements of the Methods:

3) Contraints must be implemented, either explicitly or via soft-max

4) Many methods—or aspects thereof—have a potential for improving physics analyses

5) Physics applications motivate further developments in quantification research