LAMARR
INSTITUTE FOR MACHINE LEARNING AND ARTIFICIAL INTELLIGENCE

Quantification Learning for Inverse Problems

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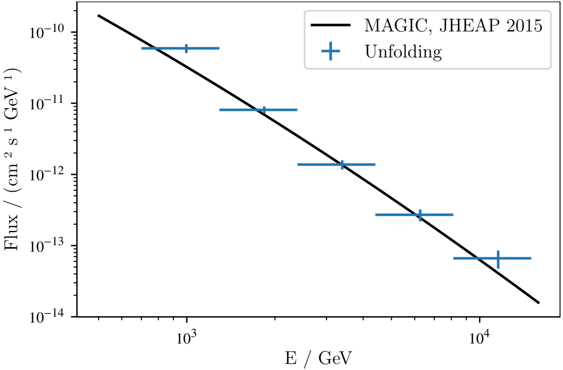
Inverse Problem: Reconstruction of Spectra

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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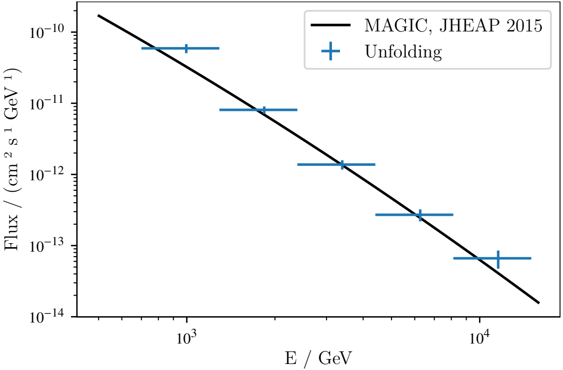
Approach: set up a linear system of equations

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



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

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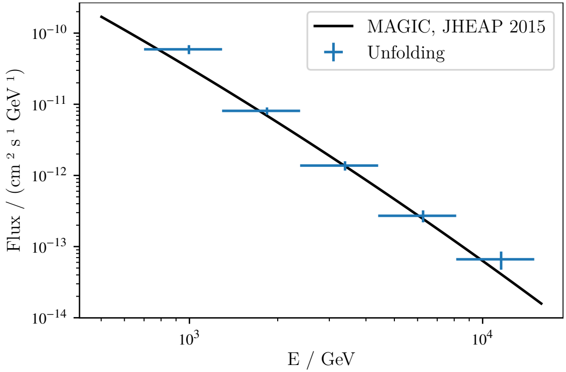

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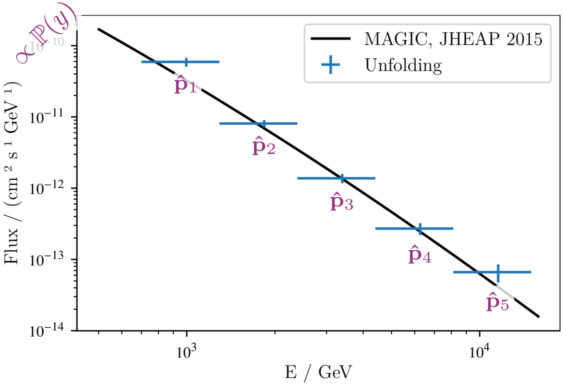

unknown $y \in [1, 5]$

$\equiv$ class label!

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Quantification

In Computer Science, this inverse problem is covered by **Quantification Learning**[2,3].

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Learn: a quantifier $\lambda : \bigcup_{m=1}^{\infty} \mathcal{X}^m \rightarrow \Delta^{C-1}$ where

- $\mathcal{X}$ is the feature space (e.g., $\mathcal{X} = \mathbb{R}^d$)
- $\Delta^{C-1} = \left\{ \mathbf{p} \in \mathbb{R}^C \; : \; \mathbf{p}_i \geq 0 \, \forall i, \; \sum_{i=1}^{C} \mathbf{p}_i = 1 \right\}$ is the space of class prevalences
- for any bag $\mathrm{B} \sim \mathbb{Q}^m$, we want to achieve that $\lambda(\mathrm{B}) = \mathbb{Q}(Y)$

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Given: a labeled training set $\mathrm{D} = \{(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}\}_{i=1}^{n} \sim \mathbb{P}^n$ where $\mathbb{P} \neq \mathbb{Q}$ (e.g., MCs)

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

} Quantification $\equiv$ Unfolding

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5 Learnings From Quantification Research

1st Learning: 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:

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

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- does not indicate good performance on finite samples
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1) RUN / TRUEE (and others) *are* Fisher consistent[4] ✓

2) DSEA & DSEA+ are *not* Fisher consistent[5] ✗

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2nd Learning: The Anatomy of Prediction Errors

Prediction Error Bound:[6] describes the *impact of* and the *interplay between* causes of errors.

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

where

- $\lambda(\mathrm{B})$ 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

6 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[7]	$\hat{\mathbf{p}} = \underset{\mathbf{p} \in \mathbb{R}^C}{\arg\min} \; \ell(\mathbf{p};\, \mathbf{q}, \mathbf{M})$	invalid: $\hat{\mathbf{p}} \notin \Delta^{C-1}$ ✗

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Soft-Max[9]	$\hat{\mathbf{p}} = \sigma(\mathbf{l}^*), \quad \mathbf{l}^* = \underset{\mathbf{l} \in \mathbb{R}^{C-1}}{\arg\min} \; \ell(\sigma(\mathbf{l});\; \mathbf{q}, \mathbf{M})$	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.

[10] Bella et al., "Quantification via Probability Estimators", 2010, .
[11] González-Castro, Alaíz-Rodríguez, and Alegre, "Class distribution estimation based on the Hellinger distance", 2013, .
[12] Börner et al., "Measurement/Simulation Mismatches and Multivariate Data Discretization in the Machine Learning Era", 2020, .
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Representations: hard[3] & soft[10] classification, histograms[11], tree-based binnings[12], kernel means[13], ...

Loss Functions: least squares[3,10], Hellinger distance[11], energy distance[13], Poisson likelihood[7], ...

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Likelihood Principle:

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[14] Alexandari, Kundaje, and Shrikumar, “Maximum Likelihood with Bias-Corrected Calibration is Hard-To-Beat at Label Shift Adaptation”, 2020.

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Maximum Likelihood Method:[14] choose $\hat{\mathbf{p}} = \arg\min_{\mathbf{p} \in \Delta^{C-1}} -\sum_{\mathbf{x} \in \mathrm{B}} \log \sum_{y \in \mathcal{Y}} \underbrace{\frac{\hat{\mathbb{P}}(y \mid \mathbf{x})}{\hat{\mathbb{P}}(y)}}_{\text{event-wise contributions}} \cdot \mathbf{p}_y$

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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])

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- data-MC mismatches / concept shift: $\mathbb{Q}(\mathbf{x} \mid y) \neq \mathbb{P}(\mathbf{x} \mid y)$ (in addition to PPS)
- inspect contributions of individual data items $\mathbf{x} \in \mathrm{B}$ to $\lambda(\mathrm{B})$ (data selection, human in the loop)

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

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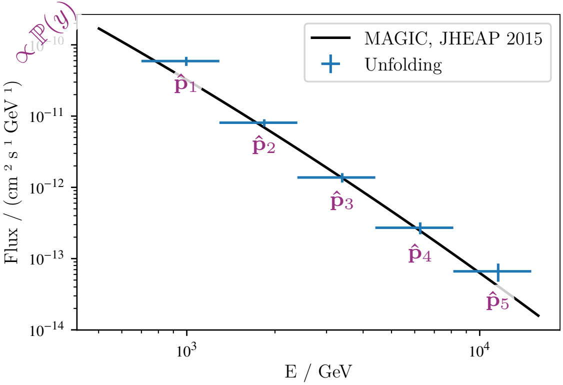

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Improvements of the Methods:

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

4) Many methods—or aspects thereof—are still to be evaluated within physics

5) Physics applications motivate further developments in quantification research