On the Role of Nonparametric Statistics in the Age of AI

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August 8, 2024

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Context

- Artificial Intelligence (AI) is emerging as an important technology

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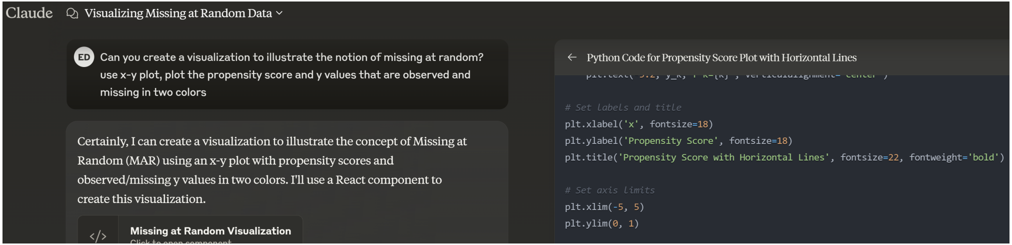
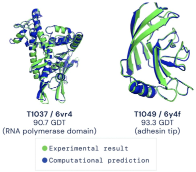
- Success stories: Large language models (ChatGPT, Claude), Image generation (Dall-E, Stable Diffusion), Protein structure prediction ...





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  - ChatGPT has 100 million weekly active users
  - Nvidia is one of the world's most valuable publicly traded companies
  - AI starting to be used in products: Code assistants (Copilot), Customer service, Web search
  - Several papers in Nature/Science reporting discoveries using AI

Article

Scaling deep learning for materials discovery

https://doi.org/10.1038/s41586-023-06735-9
Received: 8 May 2023
Accepted: 10 October 2023
Published online: 29 November 2023

Amil Merchant[1,3], Simon Batzner[1,3], Samuel S. Schoenholz[1,3], Muratahan Aykol[1], Gowoon Cheon[2] & Ekin Dogus Cubuk[1,3]

Novel functional materials enable fundamental breakthroughs across technological applications from clean energy to information processing[1–11]. From microchips to

But what is AI?

- Relies on a predictive model $\hat{p}$, such that for all $x \in \mathcal{X}$ (images, text), $\hat{p}(\cdot|x)$ is a probability distribution over a set $\mathcal{Y}$ (images, text) from which we can sample

Predictive Model $\hat{p}$	Input Space $\mathcal{X}$	Sample Space $\mathcal{Y}$
Large Language Models	Text	Text
Diffusion Models	Text	Images
Multimodal Language Models	Images, text	Images, text, sound, video
Protein Structure Prediction	Amino acid sequence	3D structure

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- Enormous engineering effort around it (input/output/UX, specialized hardware, multiple calls, ...)

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- E.g., for LLMs:
  - Data type: strings $x = (x_1, x_2, \dots, x_{\mathrm{len}(x)})$;
  - Loss: $-\sum_{x \in \mathcal{D}} \sum_{i \leq \mathrm{len}(x)} \log p_\theta(x_i | x_1, \dots, x_{i-1}) = -\sum_{x \in \mathcal{D}} \log p_\theta(x)$
  - Function class $\theta \mapsto p_\theta$: Huge neural nets
  - Dataset: Mixture of internet data sets (books, Wikipedia, arxiv, Common Crawl, ...?)

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  - Algorithmic fairness

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  - Uncertainty quantification in AI/ML
  - Algorithmic fairness
  - AI evaluation
  - ...

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Motivation

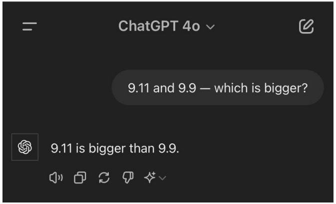
Uncertainty quantification in AI/ML

Algorithmic Fairness

AI Evaluation

Uncertainty quantification in AI/ML

- AI systems can be wrong



Uncertainty quantification in AI/ML

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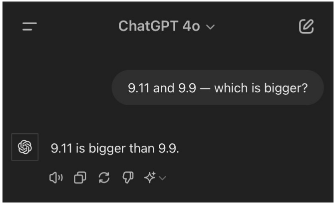

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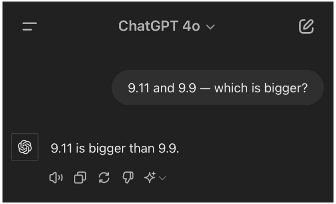

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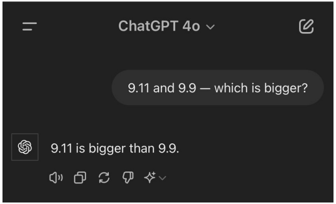

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Uncertainty in Language Models: Assessment through Rank-Calibration

Xinmeng Huang[*†] **Shuo Li**[*†] **Mengxin Yu**[†] **Matteo Sesia**[‡] **Hamed Hassani**[†]

Insup Lee[†] **Osbert Bastani**[§†] **Edgar Dobriban**[§†]

Example uncertainty measures

- Many uncertainty measures for LLMs have been discussed/proposed
  - Perplexity: $U(x, y) = \hat{p}(y|x)^{1/\mathrm{len}(y)}$; [related to NLL $-\log \hat{p}(y|x)$]

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  - Semantic entropy: generate multiple ys, cluster them based on meaning, calculate entropy (Kuhn et al., 2023)

Answers to the question "What is the capital of France?"

Answer $\mathbf{s}$	Likelihood $p(\mathbf{s} \mid x)$	Semantic likelihood $\sum_{\mathbf{s} \in c} p(\mathbf{s} \mid x)$
Paris	0.5	0.9
It's Paris	0.4	
London	0.1	0.1
Entropy	0.94	0.33

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  - Affinity graph: generate multiple ys, put pairwise similarities in a matrix, find eigenvalues/vectors (denoted EigV) (Lin et al., 2023)

Good uncertainty measures

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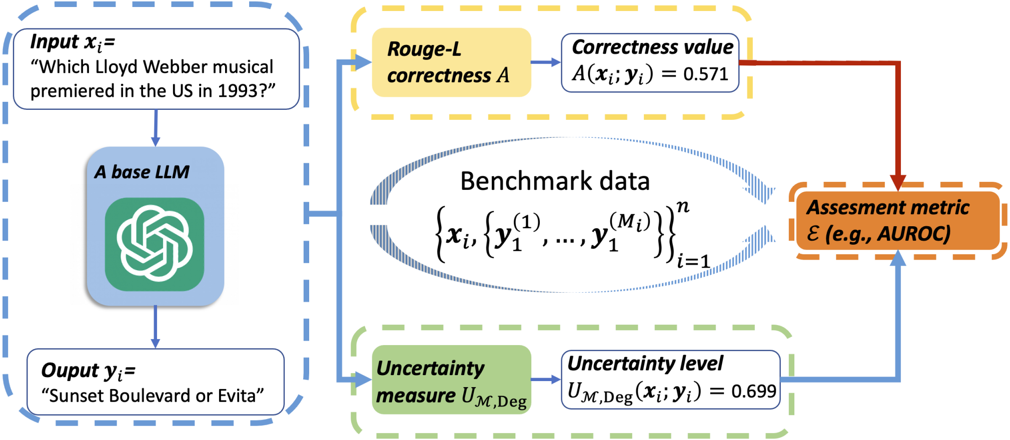

Regression function and indication diagram

- Define the regression function $\mathrm{reg}(\cdot) : \mathbb{R} \to \mathbb{R}, u \mapsto \mathbb{E}_{\boldsymbol{x},\boldsymbol{y}}[A(\boldsymbol{x}; \boldsymbol{y}) \mid U(\boldsymbol{x}; \boldsymbol{y}) = u]$, representing the *expected correctness level* A *given an uncertainty level* $U = u$.

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- Indication diagram: plot of estimated regression function as a fn. of U-percentiles.

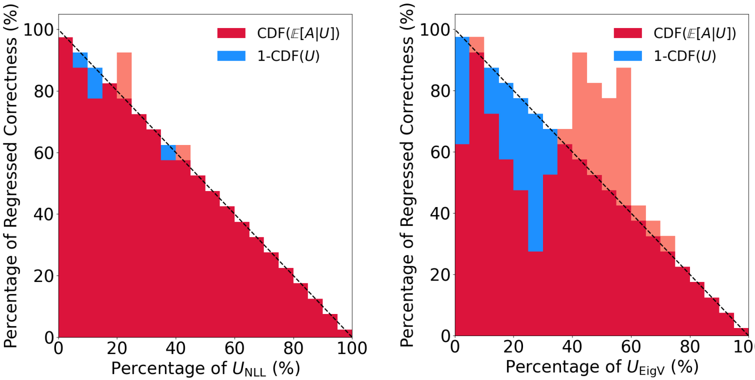
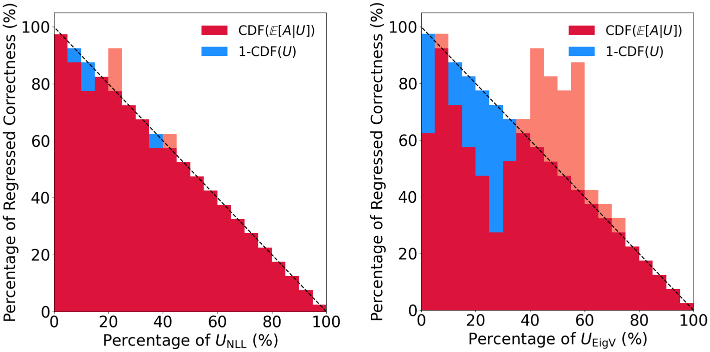


Figure: *Indication diagrams* for U_{NLL} (negative log-likelihood) and U_{EigV}, for the GPT-3.5-turbo model on the TriviaQA benchmark.

Rank-calibration

Definition (Rank-Calibration)

An uncertainty measure U is *rank-calibrated* if reg is strictly *monotone decreasing*: on average, lower uncertainty implies higher generative quality.



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Rank-calibration error (RCE)

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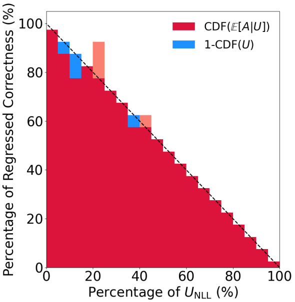
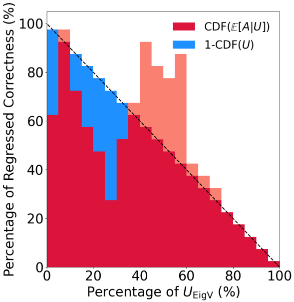
Definition (Rank-Calibration Error)

The RCE of an uncertainty measure U is defined as

$$\mathbb{E}_{U'}\left[\left|\mathbb{P}_U(U \leq U') - \mathbb{P}_U(\mathrm{reg}(U) \geq \mathrm{reg}(U'))\right|\right],$$

where U' is an independent copy of U.





Empirical results

correctness	temperature	U_{Deg}	U_{EigV}	U_{NLL}	U_{SE}
bert	0.5	$0.212_{\pm 0.040}$	$0.212_{\pm 0.041}$	$\mathbf{0.043}_{\pm 0.006}$	$0.052_{\pm 0.009}$
	1.0	$0.129_{\pm 0.020}$	$0.133_{\pm 0.020}$	$\mathbf{0.039}_{\pm 0.007}$	$0.052_{\pm 0.012}$
	1.5	$0.053_{\pm 0.011}$	$0.074_{\pm 0.012}$	$\mathbf{0.031}_{\pm 0.007}$	$0.081_{\pm 0.009}$
meteor	0.5	$0.211_{\pm 0.045}$	$0.208_{\pm 0.047}$	$\mathbf{0.179}_{\pm 0.021}$	$0.234_{\pm 0.019}$
	1.0	$0.131_{\pm 0.024}$	$\mathbf{0.131}_{\pm 0.022}$	$0.146_{\pm 0.011}$	$0.209_{\pm 0.012}$
	1.5	$\mathbf{0.059}_{\pm 0.011}$	$0.077_{\pm 0.012}$	$0.119_{\pm 0.010}$	$0.176_{\pm 0.015}$
rougeL	0.5	$0.210_{\pm 0.042}$	$0.207_{\pm 0.041}$	$\mathbf{0.041}_{\pm 0.007}$	$0.050_{\pm 0.008}$
	1.0	$0.126_{\pm 0.019}$	$0.129_{\pm 0.019}$	$\mathbf{0.038}_{\pm 0.007}$	$0.059_{\pm 0.009}$
	1.5	$0.059_{\pm 0.012}$	$0.079_{\pm 0.011}$	$\mathbf{0.034}_{\pm 0.008}$	$0.104_{\pm 0.007}$
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	1.0	$0.126_{\pm 0.018}$	$0.130_{\pm 0.021}$	$\mathbf{0.039}_{\pm 0.007}$	$0.060_{\pm 0.009}$
	1.5	$0.060_{\pm 0.011}$	$0.078_{\pm 0.012}$	$\mathbf{0.034}_{\pm 0.008}$	$0.105_{\pm 0.008}$

Table: RCE results for various experimental configurations.

Finding: models often have large rank calibration error (so uncertainty measures do not reflect performance).

Reducing RCE via re-calibration

- Re-calibrate uncertainty measure: change it to piece-wise constant estimate of regression function; Inspired by classical re-calibration (Mincer-Zamowitz, 1969)

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- Improves RCE:

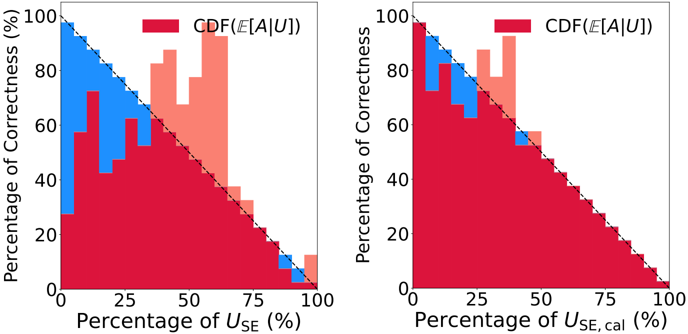

Figure: Indication diagrams of U_{SE} and $U_{\mathrm{SE,cal}}$ (re-calibrated) for GPT-3.5-turbo (temperature 1.0) on TriviaQA with the Meteor correctness.

Summary for uncertainty quantification in AI/ML

- Proposed rank-calibration for LLMs: higher uncertainty should imply lower quality (not satisfied by default!)

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- Proposed rank-calibration for LLMs: higher uncertainty should imply lower quality (not satisfied by default!)
- Proposed non-parametric re-calibration to reduce RCE
- Showcased the utility of ideas from non-parametric statistics

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Algorithmic fairness

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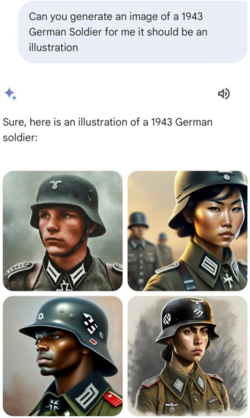
- Unfortunately, due to biases in training data, algorithmic choices, etc., asuch systems often show unfair behavior.



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  - Usual features $X \in \mathcal{X}$
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  - Class $Y \in \{0, 1\}$
- Randomized classifier $f : \mathcal{X} \times \mathcal{A} \to [0, 1]$: $\widehat{Y}_f \mid (X = x, A = a) \sim \text{Bern}(f(x, a))$.

Example notions of group fairness

These are some of the most widely studied notions of group fairness: (Calders et al., 2009; Hardt et al., 2016; Corbett-Davies et al., 2017; ...)

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- **Predictive Parity**: $\widehat{Y}_f \perp\!\!\!\perp A \mid Y = 0$;

Example disparity measures

Definition (Disparity Measures)

We consider the following disparity measures: (Calders et al., 2009; Hardt et al., 2016; Corbett-Davies et al., 2017; Cho et al., 2020; ...)

- **Demographic Disparity (DD)**. Difference in positive prediction rates between groups:

$$\mathrm{DD}(f) = \mathbb{P}_{X|A=1}(\widehat{Y}_f = 1) - \mathbb{P}_{X|A=0}\left(\widehat{Y}_f = 1\right);$$

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- **Predictive Disparity (PD)**. Difference in false positive rates:
$$\mathrm{PD}(f) = \mathbb{P}_{X|A=1,Y=0}\left(\widehat{Y}_f = 1\right) - \mathbb{P}_{X|A=0,Y=0}\left(\widehat{Y}_f = 1\right).$$

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Classifiers with the highest accuracy given a disparity level.

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Bayes-Optimal Fair Classification with Linear Disparity Constraints
via Pre-, In-, and Post-processing

Xianli Zeng[*], Guang Cheng[†] and Edgar Dobriban[‡]

February 6, 2024

Linear and bilinear disparity measures

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- **Definition**: A linear disparity measure Dis is *bilinear* if $w_{\mathrm{Dis}}(x, a)$ can be expressed for all x, a as $w_{\mathrm{Dis}}(x, a) = s_{\mathrm{Dis},a} \eta_a(x) + b_{\mathrm{Dis},a}$.
- **Proposition**: The disparity measures DD, DO, and PD are bilinear: for all x, a

$$w_{\mathrm{DD}}(x, a) = \frac{(2a-1)}{p_a}; \; w_{\mathrm{DO}}(x, a) = \frac{(2a-1)\eta_a(x)}{p_{a,1}}; \; w_{\mathrm{PD}}(x, a) = \frac{(2a-1)(1-\eta_a(x))}{p_{a,0}}.$$

Intuition for optimal fair classifiers

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- Intuitive that an optimal classifier should be of the form (for some c)

$$f(x,a) = I\left(\eta_a(x) > \frac{1}{2} + c \cdot w_{\mathrm{Dis}}(x,a)\right).$$

Optimal fair classifiers for linear and bilinear disparity measures

Consider linear disp. measure Dis; Continuous r.v.s $\eta_a(X)$, $w_{\mathrm{Dis}}(X, a)$, $a \in \{0, 1\}$.

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Theorem (Optimal Classifiers for Linear Disp. Measures; Zeng et al., 2024)

Let $t_{\mathsf{Dis}}(\delta) = \operatorname{argmin}_t\{|t| : |D_{\mathsf{Dis}}(t)| \leq \delta\}$, *where*

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A fair Bayes-optimal classifier is, for all x, a,

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If Dis *is bilinear, this is a group-wise thresholding rule, such that for all* x, a,

$$f^{\star}_{\mathrm{Dis},\delta}(x, a) = I\left(\eta_a(x) > \frac{1 + b_{\mathrm{Dis},a} \cdot t_{\mathrm{Dis}}(\delta)}{2 - s_{\mathrm{Dis},a} \cdot t_{\mathrm{Dis}}(\delta)}\right).$$

Discussion, methods, and empirics

- Proof via the *generalized Neyman-Pearson lemma*: maximizing a linear functional subject to linear constraints.

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  - In-Processing: Fair Cost-Sensitive Classification (FCSC);
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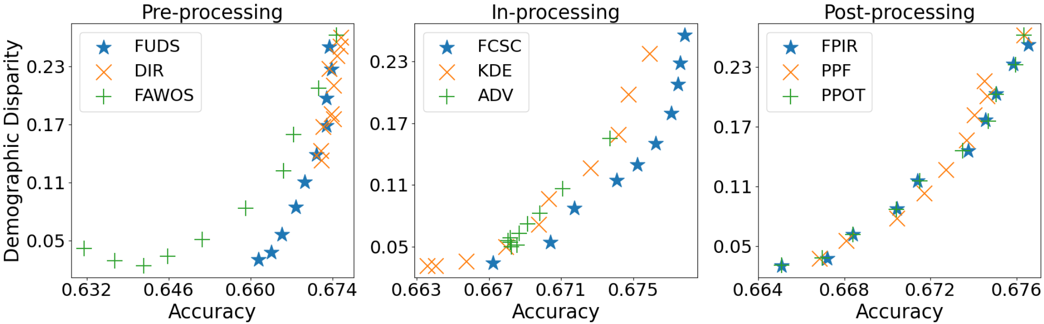

Figure: Fairness-accuracy tradeoff on the COMPAS dataset.

Summary for algorithmic fairness

- Derived fair Bayes-optimal classifiers for linear disparity measures (via Neyman-Pearson lemma!).
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- Developed fair classification methods via pre-, in-, and post-processing.
- Related work: minimax optimal fair classification.

Minimax Optimal Fair Classification
with Bounded Demographic Disparity

Xianli Zeng[*], Guang Cheng[†] and Edgar Dobriban[‡]

March 28, 2024

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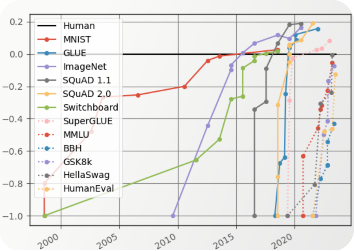

Figure: Plotting progress in AI (Kiela et al. 2023)

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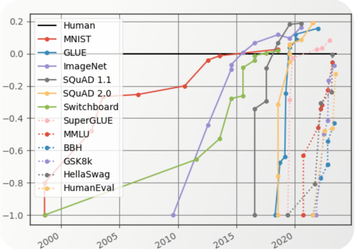

Figure: Plotting progress in AI (Kiela et al. 2023)

- Many challenges
  - Test data is necessarily arbitrary and limited
  - Correctness evaluation can be ambiguous (often use other LLMs!)
  - Evaluating the biggest models can be expensive (lots of API calls)

A statistical approach to efficient AI evaluation

tinyBenchmarks: evaluating LLMs with fewer examples

Felipe Maia Polo [1] **Lucas Weber** [2] **Leshem Choshen** [3 4] **Yuekai Sun** [1] **Gongjun Xu** [1] **Mikhail Yurochkin** [3 5]

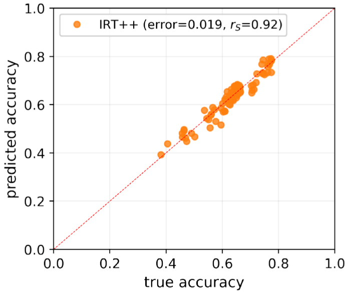

Figure 1. Estimating accuracy on MMLU (true accuracy) using 100 curated examples (predicted accuracy). IRT++, our best-performing evaluation strategy, predicts the accuracy of recent LLMs released between December 30th and January 18th within 1.9% of their true accuracy on all of MMLU (14K examples).

Item response theory (IRT) for AI evaluation

4. Better performance estimation with IRT

4.1. The IRT model

The two-parameter multidimensional IRT model assumes that the probability of the LLM j getting example i correctly is given by

$$p_{il} \triangleq \mathbb{P}(Y_{il} = 1 \mid \theta_l, \alpha_i, \beta_i) = \frac{1}{1+\exp(-\alpha_i^\top \theta_l + \beta_i)}, \quad (4.1)$$

where $\theta_l \in \mathbb{R}^d$ denotes the unobserved abilities of LLM l, while $\alpha_i \in \mathbb{R}^d$ dictates which dimensions of θ_l are required from model l to respond to example i correctly. In this formulation, $\beta_i \in \mathbb{R}$ can be viewed as a bias term that regulates the probability of correctness when $\theta_l = 0$.

Formally, we are interested in approximating

$$Z_{jl} \triangleq \frac{1}{|\mathcal{I}_j|} \sum_{i \in \mathcal{I}_j} Y_{il} \quad (4.2)$$

Now, assume that we have run model l on a subset of examples from scenario j, obtaining responses $\{Y_{i_0 l}, \cdots, Y_{i_k l}\}$ for the examples $\widehat{\mathcal{I}}_j = \{i_0, \cdots, i_k\}$. Let $\widehat{\theta}_l$ denote the estimate for θ_l after observing $\widehat{\mathcal{I}}_j$ and possibly a bigger set of examples coming from different scenarios. To obtain that estimate, we maximize the log-likelihood of the freshly observed data with respect to θ_l, fixing examples' parameters. This procedure is equivalent to fitting a logistic regression model.

Because Z_{jl} is a random variable, we approximate it by estimating the conditional expectation

$$\mathbb{E}[Z_{jl} \mid Y_{i_0 l}, \cdots, Y_{i_k l}] = \\ = \frac{1}{|\mathcal{I}_j|} \sum_{i \in \mathcal{I}_j} \mathbb{E}[Y_{il} \mid Y_{i_0 l}, \cdots, Y_{i_k l}]$$

The probability $p_{il} = \mathbb{P}(Y_{il} = 1 \mid \theta_l, \alpha_i, \beta_i)$ is given by the IRT model in Equation 4.1. The estimator for the conditional expectation is then given by

$$\hat{Z}_{jl}^{\text{p-IRT}} \triangleq \widehat{\mathbb{E}}[Z_{jl} \mid Y_{i_0 l}, \cdots, Y_{i_k l}] \quad (4.3) \\ = \frac{\hat{\lambda}}{|\widehat{\mathcal{I}}_j|} \sum_{i \in \widehat{\mathcal{I}}_j} Y_{il} + \frac{1-\hat{\lambda}}{|\mathcal{I}_j \setminus \widehat{\mathcal{I}}_j|} \sum_{i \in \mathcal{I}_j \setminus \widehat{\mathcal{I}}_j} \hat{p}_{il}$$

where $\hat{p}_{il} \triangleq \mathbb{P}(Y_{il} = 1 \mid \widehat{\theta}_l, \widehat{\alpha}_i, \widehat{\beta}_i)$.

Summary and outlook

- We explored and illustrated how (nonparametric) statistics could have an impact in the world of AI. The most exciting discoveries are yet to come!
- Thanks!