

On the Role of Nonparametric Statistics in the Age of AI

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Uncertainty quantification in AI/ML

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AI Evaluation

Context

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- ▶ Success stories: Large Language Models (ChatGPT, Claude), Generative AI (Dall-E, Stable Diffusion), Protein structure prediction ...

Claude Q Visualizing Missing at Random Data ▾

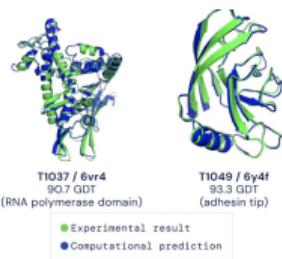
ED Can you create a visualization to illustrate the notion of missing at random? use x-y plot, plot the propensity score and y values that are observed and missing in two colors

Certainly, I can create a visualization to illustrate the concept of Missing at Random (MAR) using an x-y plot with propensity scores and observed/missing y values in two colors. I'll use a React component to create this visualization.

</> Missing at Random Visualization
Click to open component

```
← Python Code for Propensity Score Plot with Horizontal Lines
plt.scatter(x=x, y=y, c=c, s=s, edgecolor='black', linewidth=1, alpha=0.8)
plt.xlabel('x', fontsize=18)
plt.ylabel('Propensity Score', fontsize=18)
plt.title('Propensity Score with Horizontal Lines', fontsize=22, fontweight='bold')

# Set axis limits
plt.xlim(-5, 5)
plt.ylim(0, 1)
```



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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

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Amil Merchant^{1,3}✉, Simon Batzner^{1,3}, Samuel S. Schoenholz^{1,3}, Muratahan Aykol¹,

Gwoon Cheon² & 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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- ▶ The predictive model \hat{p} is obtained by minimizing a simple **loss function** over a **non-parametric function class** using a **massive data set**
- ▶ E.g., for LLMs:
 - ▶ Data: strings $x = (x_1, x_2, \dots, x_{\text{len}(x)})$
 - ▶ Loss: $-\sum_{x \in \mathcal{D}} \sum_{i \leq \text{len}(x)} \log p_\theta(x_i | x_1, \dots, x_{i-1}) = -\sum_{x \in \mathcal{D}} \log p_\theta(x)$
 - ▶ Function class $\theta \mapsto p_\theta$: Huge neural nets
 - ▶ Dataset: Mixture of Internet data sets (books, Wikipedia, arxiv, Common Crawl, ...?)

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- ▶ Will discuss a few emerging areas of research where statistics could have an impact:
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 - ▶ Algorithmic fairness
 - ▶ AI evaluation
 - ▶ ...

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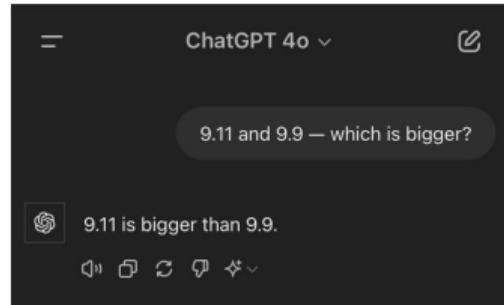
Uncertainty quantification in AI/ML

Algorithmic Fairness

AI Evaluation

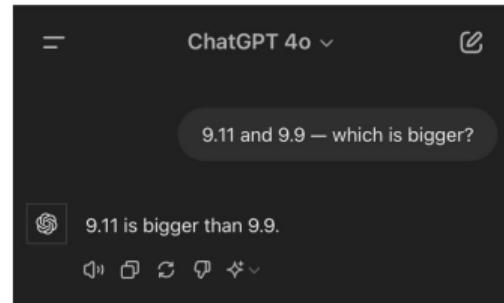
Uncertainty quantification in AI/ML

- ▶ AI systems can be wrong



Uncertainty quantification in AI/ML

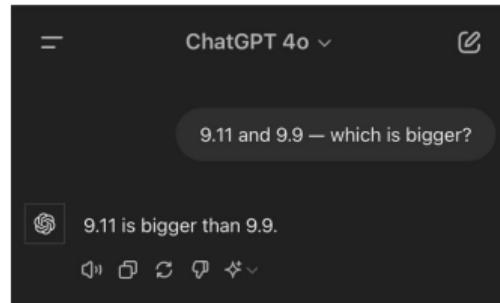
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- ▶ One emerging idea: Quantify uncertainty (and then perhaps refrain from generating when it is high)

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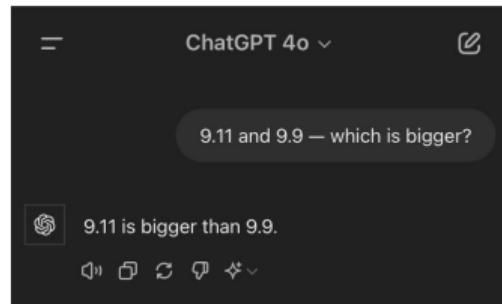
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- ▶ But what does it mean to quantify uncertainty? and what properties does good uncertainty quantification have?

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- ▶ One emerging idea: Quantify uncertainty (and then perhaps refrain from generating when it is high)
- ▶ But what does it mean to quantify uncertainty? and what properties does good uncertainty quantification have?

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: $U(x, y) = \hat{p}(y|x)^{1/\text{len}(y)}$; [related to NLL – $\log \hat{p}(y|x)$]

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

Answers to the question “What is the capital of France?”

Answer s	Likelihood $p(s x)$	Semantic likelihood $\sum_{s \in c} p(s x)$
Paris	0.5	0.9
It's Paris	0.4	
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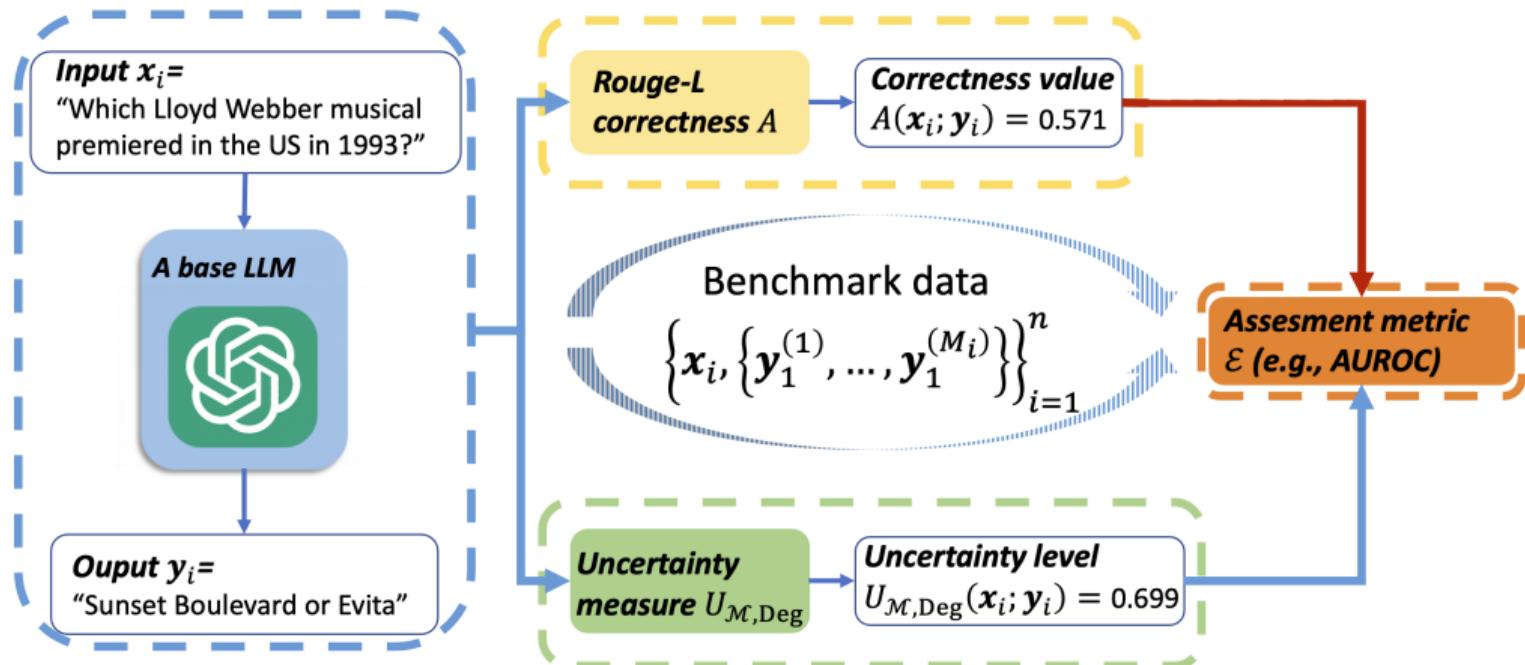
- ▶ Affinity graph: generate multiple ys, put pairwise similarities in a matrix, find eigenvalues/vectors (denoted EigV) (Lin et al., 2023)

Good uncertainty measures

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Regression function and indication diagram

- ▶ Define the **regression function** $\text{reg}(\cdot) : \mathbb{R} \rightarrow \mathbb{R}$, $u \mapsto \mathbb{E}_{\mathbf{x}, \mathbf{y}}[A(\mathbf{x}; \mathbf{y}) \mid U(\mathbf{x}; \mathbf{y}) = u]$, 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.

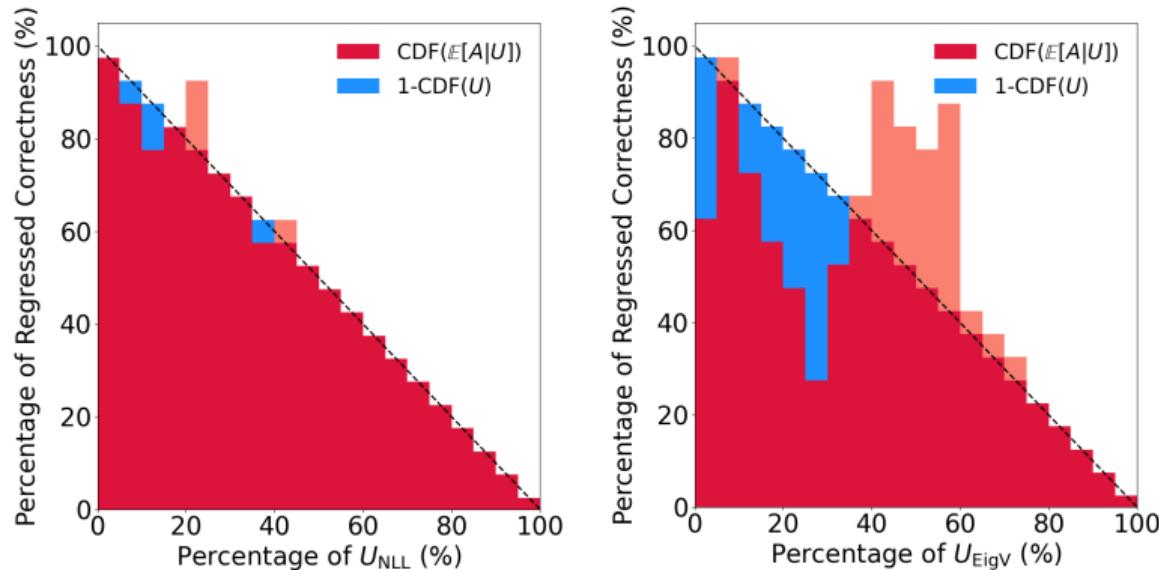


Figure: Indication diagrams for U_{NLL} (negative log-likelihood) and U_{EigV} , for the GPT-3.5-turbo model on the TriviaQA benchmark.

Rank-calibration

Definition (RANK-CALIBRATION)

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

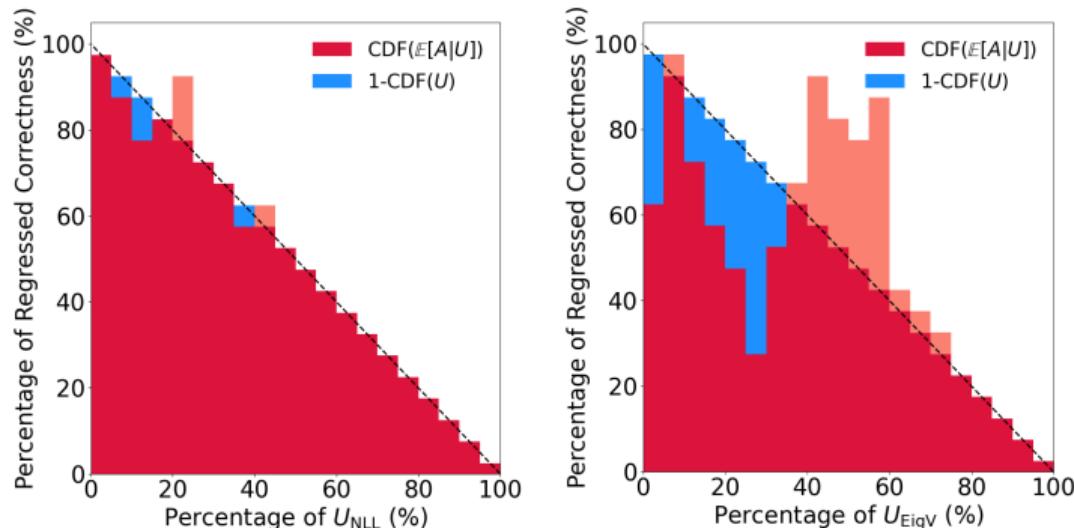


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Rank-calibration error (RCE)

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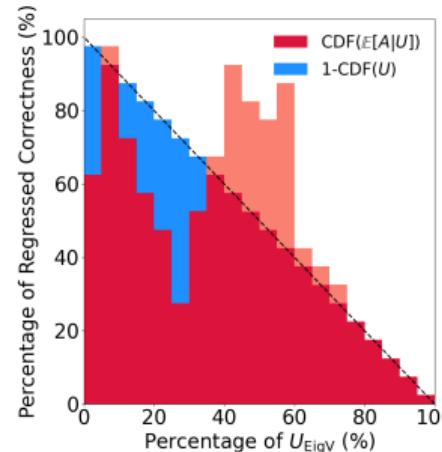
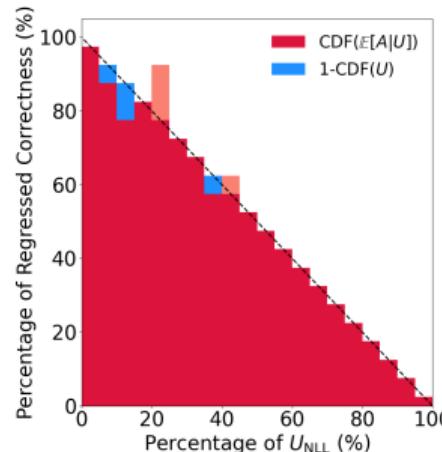
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Definition (RANK-CALIBRATION ERROR)

The RCE of an uncertainty measure U is defined as

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

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 ± 0.040	0.212 ± 0.041	0.043 ± 0.006	0.052 ± 0.009
	1.0	0.129 ± 0.020	0.133 ± 0.020	0.039 ± 0.007	0.052 ± 0.012
	1.5	0.053 ± 0.011	0.074 ± 0.012	0.031 ± 0.007	0.081 ± 0.009
meteor	0.5	0.211 ± 0.045	0.208 ± 0.047	0.179 ± 0.021	0.234 ± 0.019
	1.0	0.131 ± 0.024	0.131 ± 0.022	0.146 ± 0.011	0.209 ± 0.012
	1.5	0.059 ± 0.011	0.077 ± 0.012	0.119 ± 0.010	0.176 ± 0.015
rougeL	0.5	0.210 ± 0.042	0.207 ± 0.041	0.041 ± 0.007	0.050 ± 0.008
	1.0	0.126 ± 0.019	0.129 ± 0.019	0.038 ± 0.007	0.059 ± 0.009
	1.5	0.059 ± 0.012	0.079 ± 0.011	0.034 ± 0.008	0.104 ± 0.007
rouge1	0.5	0.212 ± 0.043	0.209 ± 0.042	0.040 ± 0.007	0.050 ± 0.008
	1.0	0.126 ± 0.018	0.130 ± 0.021	0.039 ± 0.007	0.060 ± 0.009
	1.5	0.060 ± 0.011	0.078 ± 0.012	0.034 ± 0.008	0.105 ± 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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- ▶ Re-calibrate uncertainty measure: change it to piece-wise constant estimate of regression function; Inspired by classical re-calibration (Mincer-Zamowitz, 1969)
- ▶ Improves RCE:

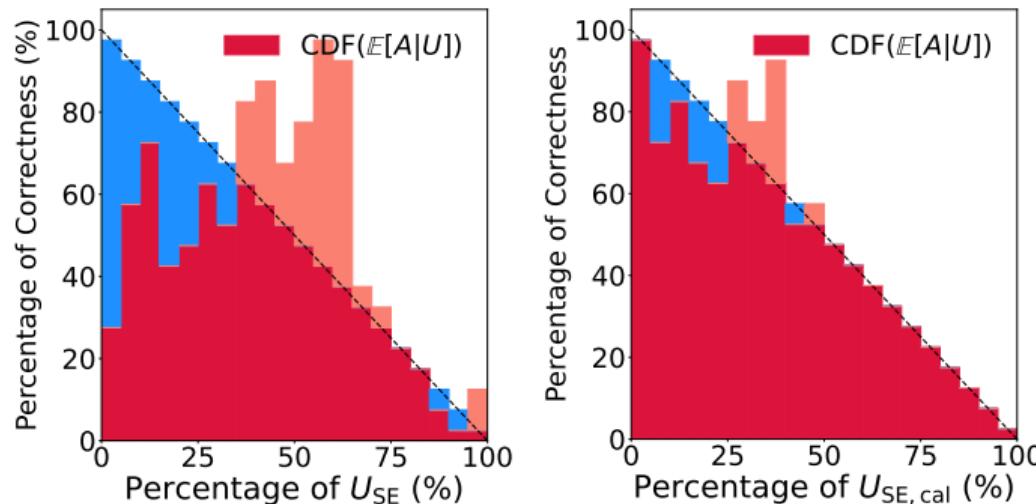


Figure: Indication diagrams of U_{SE} and $U_{SE,cal}$ (re-calibrated) for GPT-3.5-turbo (temperature 1.0) on TriviaQA with the Meteor correctness.

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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Summary for uncertainty quantification in AI/ML

- ▶ 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

Uncertainty in Language Models: Assessment through Rank-Calibration

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AI Evaluation

Algorithmic fairness

- ▶ Ensuring that AI/ML systems are fair and do not discriminate is important.

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- ▶ Ensuring that AI/ML systems are fair and do not discriminate is important.
- ▶ Unfortunately, due to biases in training data, algorithmic choices, etc., as such systems often show unfair behavior.

The screenshot shows a news article from propublica.org. At the top, there are zoom and refresh icons, followed by the URL 'propublica.org'. Below the URL is the ProPublica logo and social media links for Facebook, Twitter, and a red 'Donate' button. The main image features two men of different ethnicities side-by-side. The title 'Machine Bias' is prominently displayed in large white text. Below the title, a subtitle reads: 'There's software used across the country to predict future criminals. And it's biased against blacks.' The author's name, 'by Julia Angwin, Jeff Larson, Surya Mattu and Lauren Kirchner, ProPublica', and the date 'May 23, 2016' are at the bottom.

Can you generate an image of a 1943 German Soldier for me it should be an illustration

Sure, here is an illustration of a 1943 German soldier:



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- ▶ Fair binary classification with a binary protected attribute:
 - ▶ Usual features $X \in \mathcal{X}$
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 - ▶ Class $Y \in \{0, 1\}$
- ▶ Randomized classifier $f : \mathcal{X} \times \mathcal{A} \rightarrow [0, 1]$: $\hat{Y}_f \mid (X = x, A = a) \sim \text{Bern}(f(x, a))$.

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; ...)

- ▶ **Demographic Parity:** $\hat{Y}_f \perp\!\!\!\perp A$;

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- ▶ **Predictive Parity:** $\hat{Y}_f \perp\!\!\!\perp A | Y = 0$;

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:

$$\text{DD}(f) = \mathbb{P}_{X|A=1}(\hat{Y}_f = 1) - \mathbb{P}_{X|A=0}(\hat{Y}_f = 1);$$

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- ▶ **Disparity of Opportunity (DO)**. Difference in true positive rates:

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- ▶ **Predictive Disparity (PD)**. Difference in false positive rates:

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Fair Bayes-optimal classifiers

Classifiers with the highest accuracy given a disparity level.

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Consider any $K \geq 1$ fairness measures $\text{Dis}_k : \mathcal{F} \rightarrow [0, 1]$, $k = 1, \dots, K$. Then, a δ -fair Bayes-optimal classifier $f_{\text{Dis}, \delta}^*$ minimizes the misclassification error $R(f) := \mathbb{P}(Y \neq \hat{Y}_f)$ over all classifiers that satisfy δ -disparity:

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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 $w_{\text{Dis}}(x, a)$ can be expressed for all x, a as $w_{\text{Dis}}(x, a) = s_{\text{Dis}, a} \eta_a(x) + b_{\text{Dis}, a}$.

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$$\text{Dis}(f) = \int_{\mathcal{A}} \int_{\mathcal{X}} f(x, a) w_{\text{Dis}}(x, a) d\mathbb{P}_{X, A}(x, a).$$

- ▶ Class-conditional probability function η_a : $\eta_a(x) = \mathbb{P}(Y = 1 \mid A = a, X = x)$ for all x, a .
- ▶ **Definition:** A linear disparity measure Dis is *bilinear* if $w_{\text{Dis}}(x, a)$ can be expressed for all x, a as $w_{\text{Dis}}(x, a) = s_{\text{Dis}, a} \eta_a(x) + b_{\text{Dis}, a}$.
- ▶ **Proposition:** The disparity measures DD, DO, and PD are bilinear: for all x, a

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

Intuition for optimal fair classifiers

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s.t. $|\text{Dis}(f)| \leq \delta$

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

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

Optimal fair classifiers for linear and bilinear disparity measures

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

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

$$D_{\text{Dis}}(t) = \int_{\mathcal{X} \times \mathcal{A}} w_{\text{Dis}}(x, a) \cdot I\left(\eta_a(x) > \frac{1}{2} + \frac{t}{2} w_{\text{Dis}}(x, a)\right) d\mathbb{P}_{X,A}(x, a).$$

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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 ,

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

Discussion, methods, and empirics

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 - ▶ Pre-processing: up-& down-sampling (FUDS);
 - ▶ In-Processing: Fair Cost-Sensitive Classification (FCSC);
 - ▶ Post-Processing: Fair Plug-in Thresholding Rule (FPIR).

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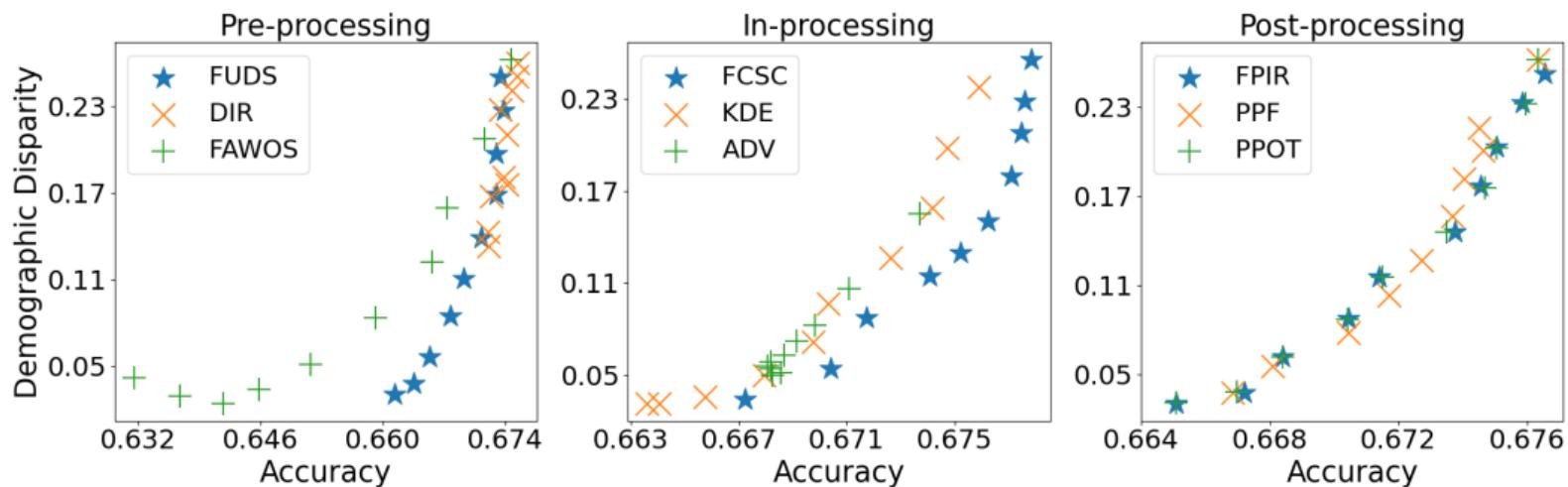


Figure: Fairness-accuracy tradeoff on the COMPAS dataset.

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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Uncertainty quantification in AI/ML

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AI Evaluation

AI evaluation

- ▶ Evaluating AI can be hard

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- ▶ Say want to measure *reasoning ability*:
 - ▶ Collect test data on reasoning problems (e.g., high school math)
 - ▶ Evaluate error rate

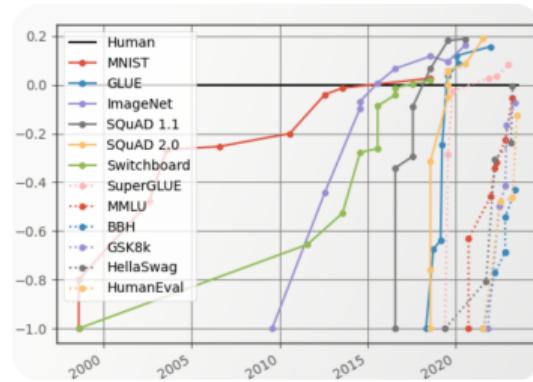


Figure: Plotting progress in AI (Kiel et al. 2023)

- ▶ 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 Polo¹ Lucas Weber² Leshem Choshen^{3,4} Yuekai Sun¹ Gongjun Xu¹ Mikhail Yurochkin^{3,5}

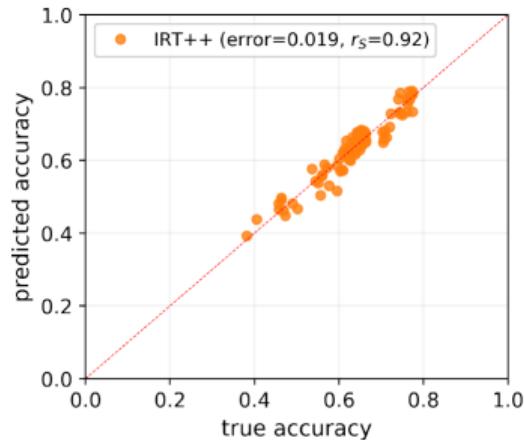


Figure 1. Estimating accuracy on MMLU (true accuracy) using 100 curated examples (predicted accuracy). IRT++, our best-performing evaluation strategy, predicts the accuracy of recent LLMs released between December 30th and January 18th within 1.9% of their true accuracy on all of MMLU (14K examples).

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 $\{Y_{i_0l}, \dots, Y_{i_kl}\}$ for the examples $\hat{\mathcal{I}}_j = \{i_0, \dots, i_k\}$. Let $\hat{\theta}_l$ denote the estimate for θ_l after observing $\hat{\mathcal{I}}_j$ 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

$$\begin{aligned} \mathbb{E}[Z_{jl} \mid Y_{i_0l}, \dots, Y_{i_kl}] &= \\ &= \frac{1}{|\mathcal{I}_j|} \sum_{i \in \mathcal{I}_j} \mathbb{E}[Y_{il} \mid Y_{i_0l}, \dots, Y_{i_kl}] \end{aligned}$$

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

$$\begin{aligned} \hat{Z}_{jl}^{\text{p-IRT}} &\triangleq \hat{\mathbb{E}}[Z_{jl} \mid Y_{i_0l}, \dots, Y_{i_kl}] \\ &= \frac{\hat{\lambda}}{|\hat{\mathcal{I}}_j|} \sum_{i \in \hat{\mathcal{I}}_j} Y_{il} + \frac{1 - \hat{\lambda}}{|\mathcal{I}_j \setminus \hat{\mathcal{I}}_j|} \sum_{i \in \mathcal{I}_j \setminus \hat{\mathcal{I}}_j} \hat{p}_{il} \end{aligned} \quad (4.3)$$

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

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!



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