



NEURAL INFORMATION
PROCESSING SYSTEMS

Uncertainty Calibration for Ensemble-Based Debiasing Methods

Ruixin Xiong*, Yimeng Chen*, Liang Pang, Xueqi Cheng, Zhiming Ma,
Yanyan Lan



Contents

- Background
- Motivation
- Method and Experiments
- Conclusion

Contents

- Background
 - Why debiasing?
 - Ensemble-based Debiasing Methods
- Motivation
- Method and Experiments
- Conclusion and Future Work

The Impressive Performance of ML Models

| Model | Accuracy | |
|-------------------------------|----------|--------------|
| | Train | Test |
| Human Performance (Estimated) | 97.2% | 87.7% |
| DR-BiLSTM (Single) | 94.1% | 88.5% |
| DR-BiLSTM (Single)+Process | 94.1% | 88.9% |
| DR-BiLSTM (Ensemble) | 94.8% | 89.3% |
| DR-BiLSTM (Ensem.)+Process | 94.8% | 89.6% |

Natural Language Inference

Even outperform human on the SNLI dataset



Identify signs of diabetic retinopathy (糖尿病视网膜病变)

> 90% accuracy (comparable with experts),
< 10 minutes¹ v.s. 1 month (human)
(By Google Health)

Failures in Real Applications

- When ML models went out of the training environment, significant drop in performance occurs
- New evidence, from Andrew Ng.

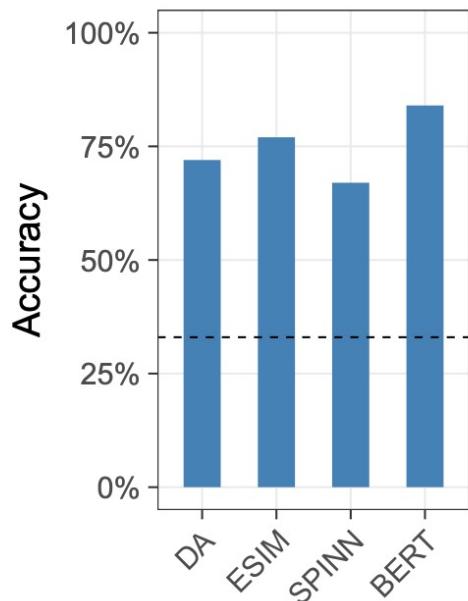
<https://spectrum.ieee.org/andrew-ng-xrays-the-ai-hype>

“It turns out [that when] you take that same model, that same AI system, to an older hospital down the street, with an older machine, and the technician uses a slightly different imaging protocol, that data drifts to cause the performance of AI system to degrade significantly. In contrast, any human radiologist can walk down the street to the older hospital and do just fine. ...”

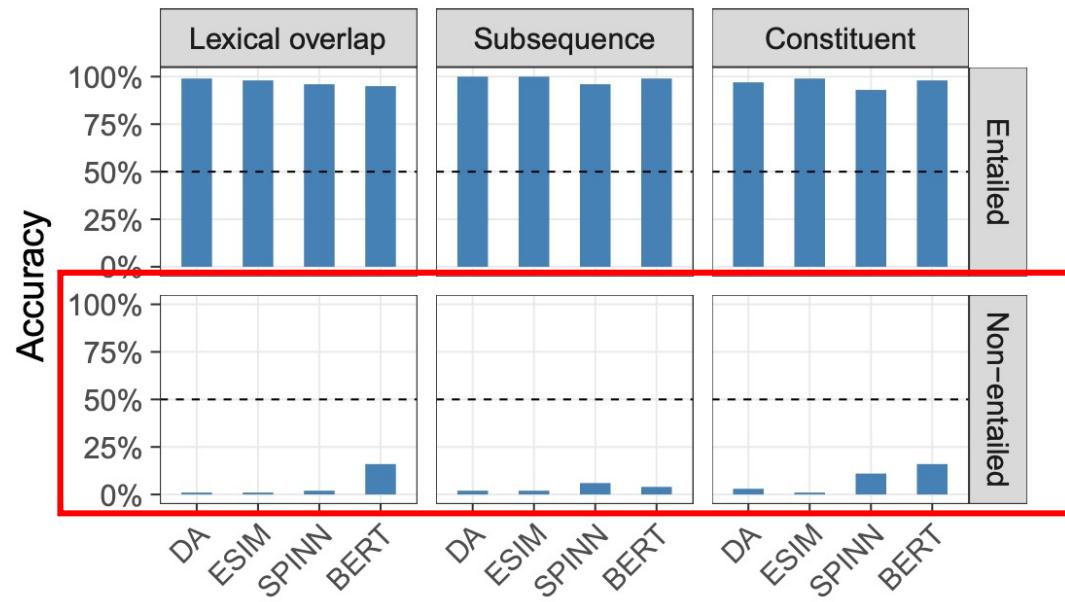
“All of AI, not just healthcare, has a proof-of-concept-to-production gap,” he says. “The full cycle of a machine learning project is not just modeling. It is finding the right data, deploying it, monitoring it, feeding data back [into the model], showing safety—doing all the things that need to be done [for a model] to be deployed. [That goes] beyond doing well on the test set, which fortunately or unfortunately is what we in machine learning are great at.”

Failures in Real Applications

- When ML models went out of the training environment, significant drop in performance occurs



Performance on MNLI



Performance on HANS

Failures in Real Applications

- When ML models went out of the training environment, significant drop in performance occurs



Identify signs of diabetic retinopathy (糖尿病视网膜病变)

> 50% images in poor lighting conditions were rejected, even no pattern of disease

Failures in Real Applications

- When ML models went out of the training environment, significant drop in performance occurs



Detect COVID-19 by CXR and CT

None of 62 machine learning models is of potential clinical use

“Any machine learning algorithm is only as good as the data it’s trained on.”

Challenges of ML in the Application

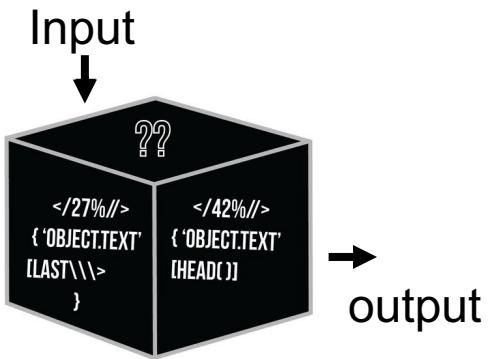
Generalizability



> 50% images in poor lighting conditions were rejected

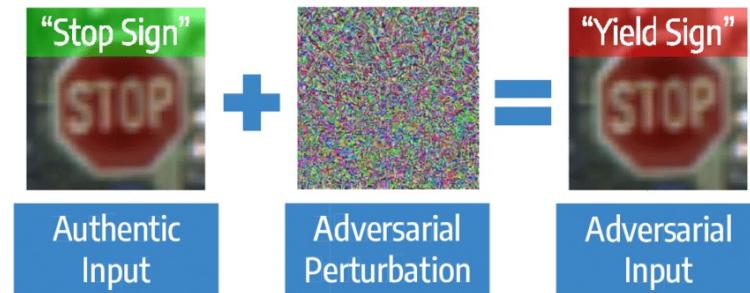
Poor performance in OOD (out-of-distribution)

Interpretability



Deep NN remains a black box to human

Robustness



Sensitive to the noise and easy to attack

Decades Efforts on These Problems

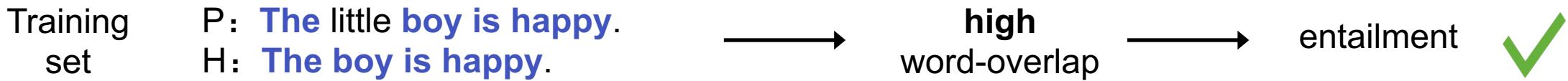
- Methods combating these problems including
 - Transfer learning
 - Data augmentation
 - Robust training
 - Causal machine learning
 - **Debiasing**
 -

What is Debiasing?

The Dependence on Spurious Correlations (Dataset Bias)

- Debiasing: to mitigate model's reliance on **Dataset bias**

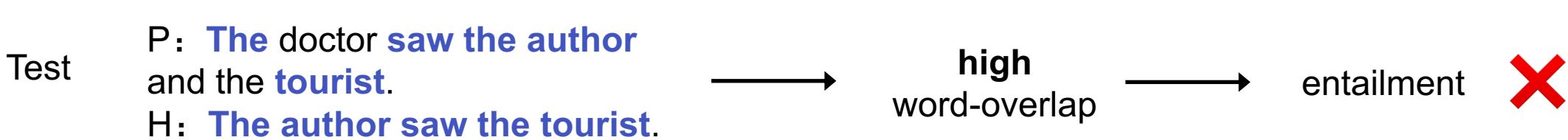
| Bias features | Heuristic | Supporting Cases | Contradicting Cases | “Entailment” “Neutral” “Contradiction” |
|---------------|-----------------|------------------|---------------------|--|
| | | | | |
| | Lexical overlap | 2,158 | 261 | |
| | Subsequence | 1,274 | 72 | |
| | Constituent | 1,004 | 58 | |



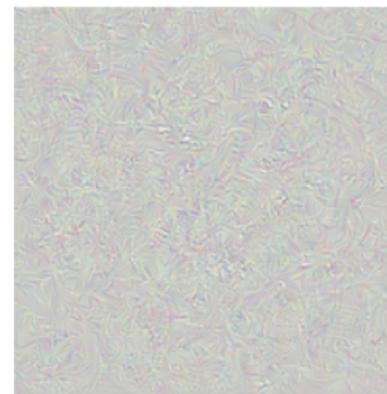
The Dependence on Spurious Correlations (Dataset Bias)

- Debiasing: to mitigate model's reliance on **Dataset bias**

| Heuristic | Supporting Cases | Contradicting Cases |
|-----------------|------------------|---------------------|
| Lexical overlap | 2,158 | 261 |
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| Constituent | 1,004 | 58 |



The Dependence on Spurious Correlations (Dataset Bias)

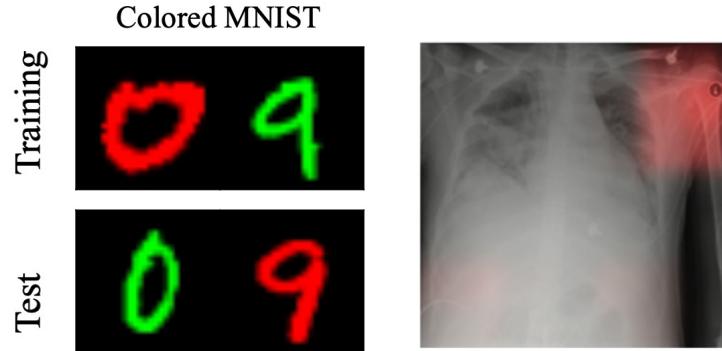


Article: Super Bowl 50
Paragraph: "Peyton Manning became the first quarterback ever to lead two different teams to multiple Super Bowls. He is also the oldest quarterback ever to play in a Super Bowl at age 39. The past record was held by John Elway, who led the Broncos to victory in Super Bowl XXXIII at age 38 and is currently Denver's Executive Vice President of Football Operations and General Manager. Quarterback Jeff Dean had a jersey number 37 in Champ Bowl XXXIV."
Question: "What is the name of the quarterback who was 38 in Super Bowl XXXIII?"
Original Prediction: John Elway
Prediction under adversary: Jeff Dean

| Task | Caption image | Recognise object | Recognise pneumonia | Answer question |
|---------|---|---|-----------------------------------|---|
| Problem | Describes green hillside as grazing sheep | Hallucinates teapot if certain patterns are present | Fails on scans from new hospitals | Changes answer if irrelevant information is added |
| Bias | Uses background to recognise primary object | Uses features irreducible to humans | Looks at hospital token, not lung | Only looks at last sentence and ignores context |

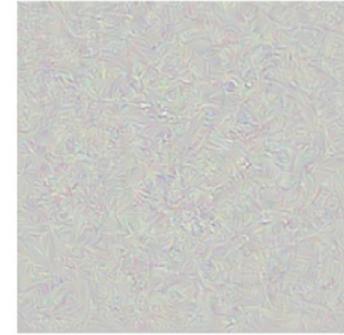
The Effects of Spurious Correlation

Generalizability



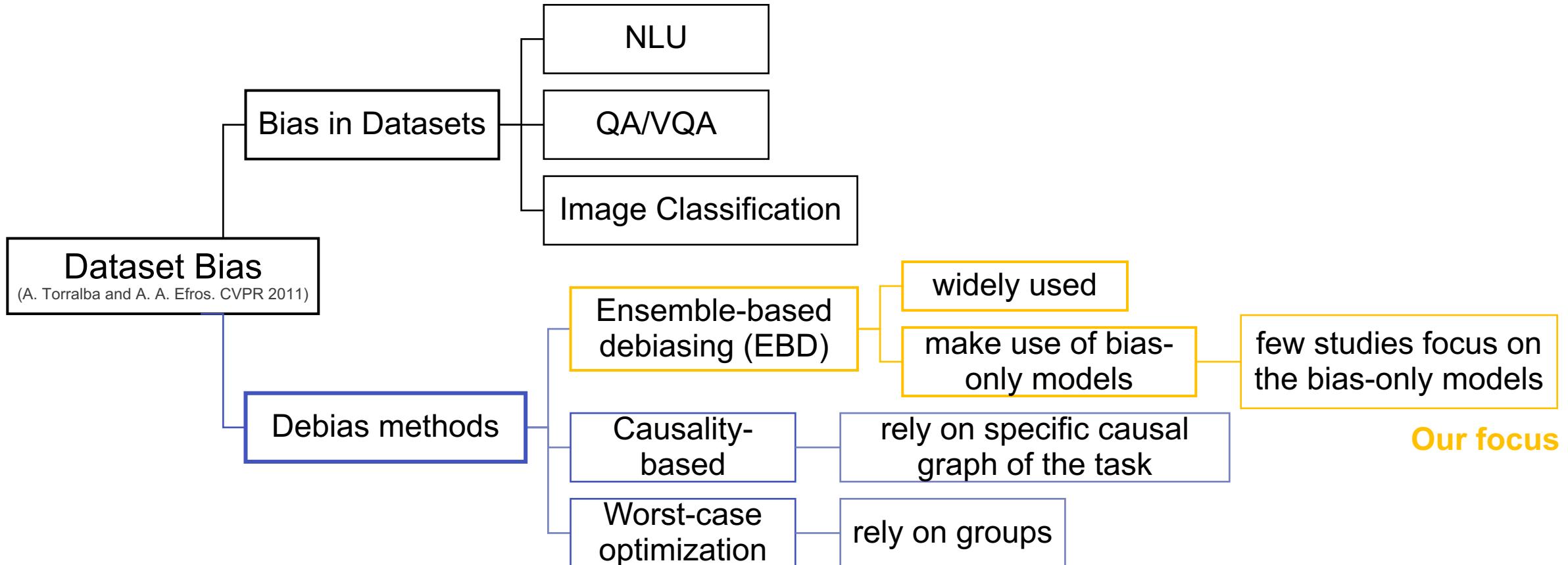
Spurious correlations are prone to change on the test set

Interpretability & Robustness

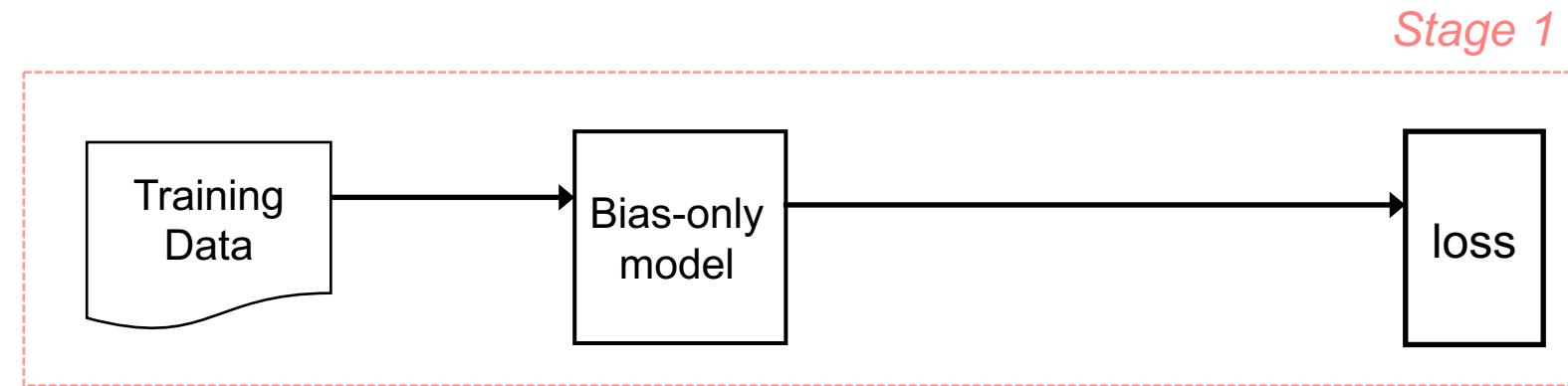


Use features unrecognizable to humans

Debiasing: reliance the effect of Dataset Bias

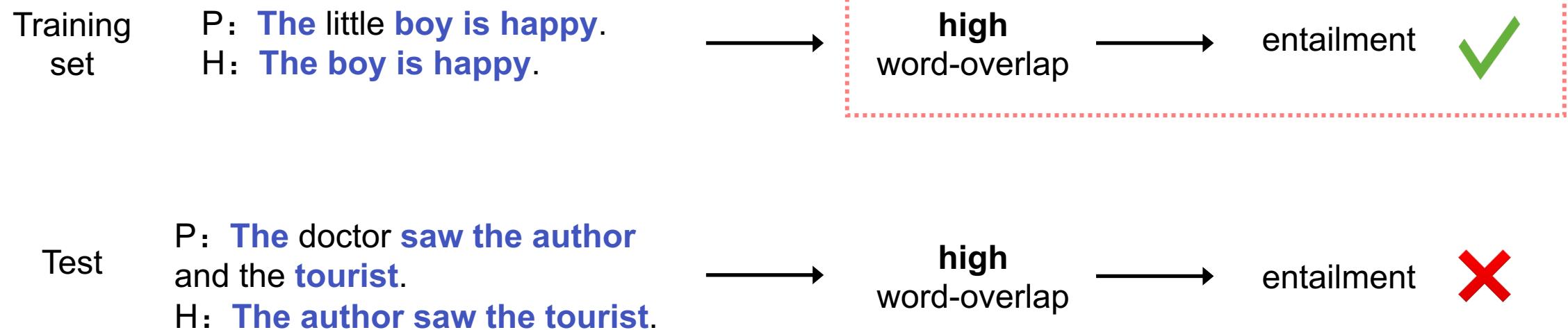


Ensemble-based Debiasing Framework



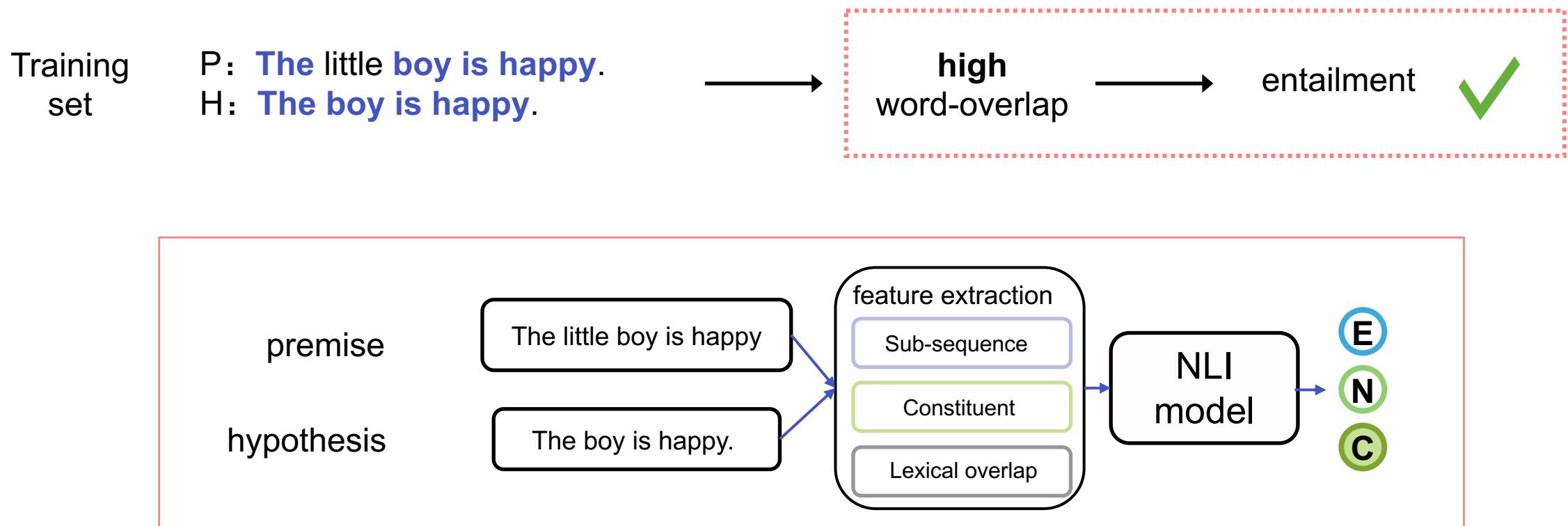
Ensemble-based Debiasing - Example

- Debiasing: to mitigate model's reliance on **Dataset bias**



Ensemble-based Debiasing - Example

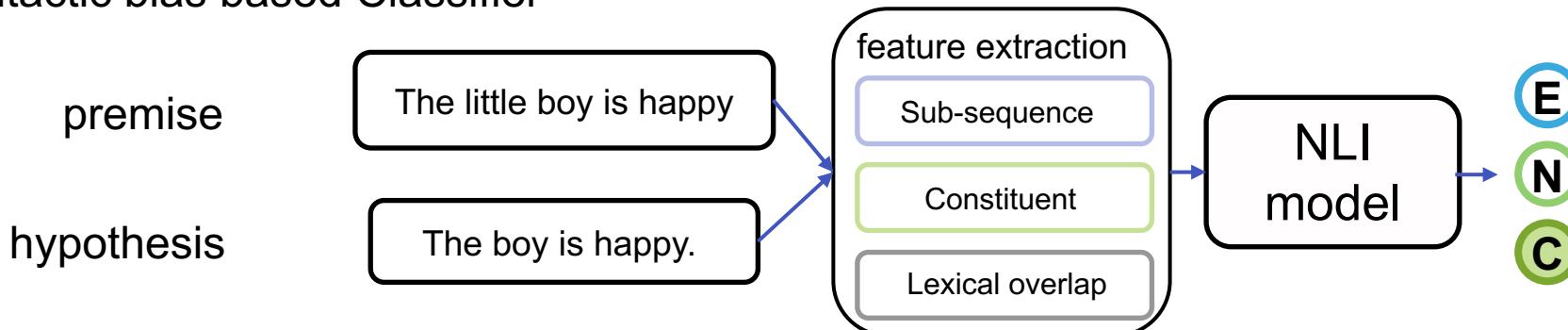
- Use a bias-only model



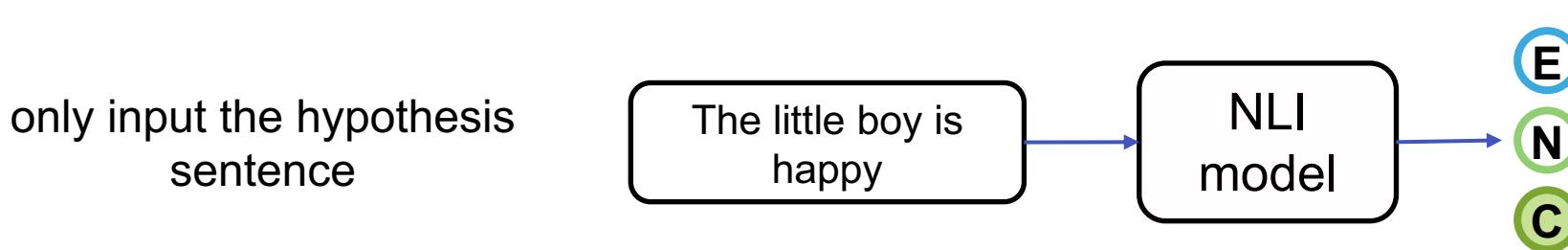
Bias-only Models

- Bias-Known: we have prior knowledge about bias features

- Syntactic bias based Classifier



- Hypothesis-only Classifier

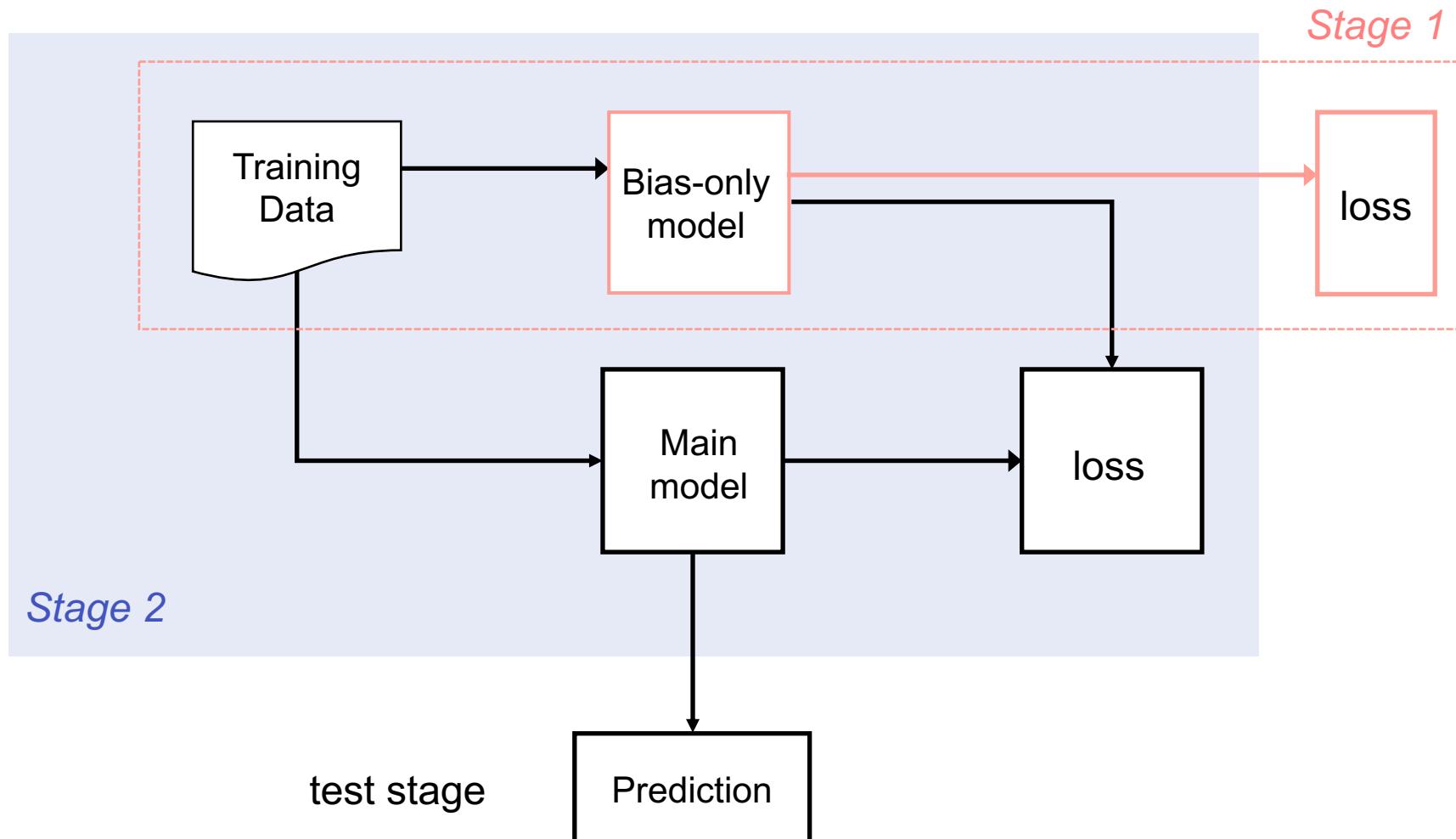


Improvements on Bias-only Models

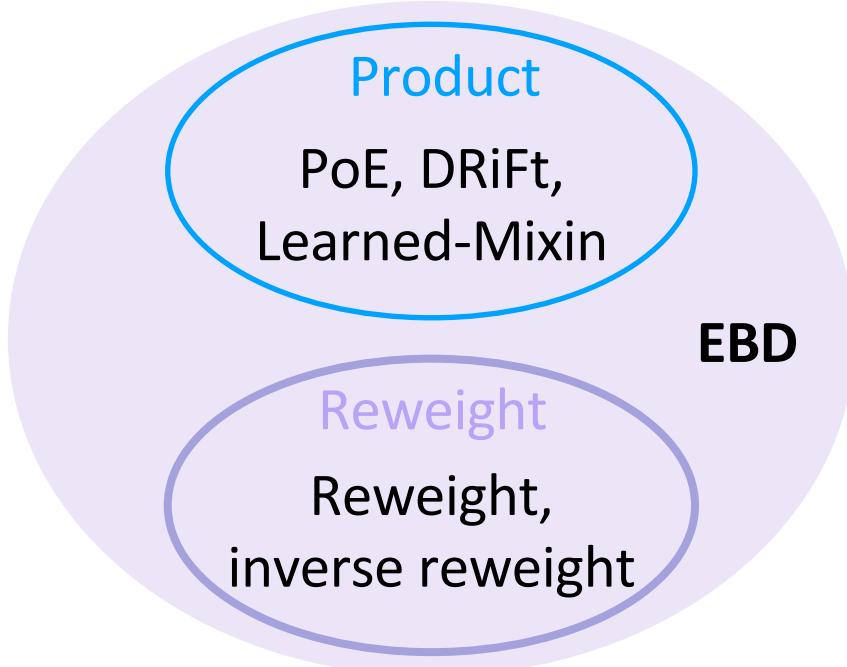
- Bias-Unknown: no identified bias features, using other assumptions
 - Low-capacity model (Clark et al. 2020)
“short-cuts”
 - Early-stage model (Utama et al. 2020)

Previous work focus on dataset bias other than bias-only model itself

Ensemble-based Debiasing Framework



Ensemble Strategies



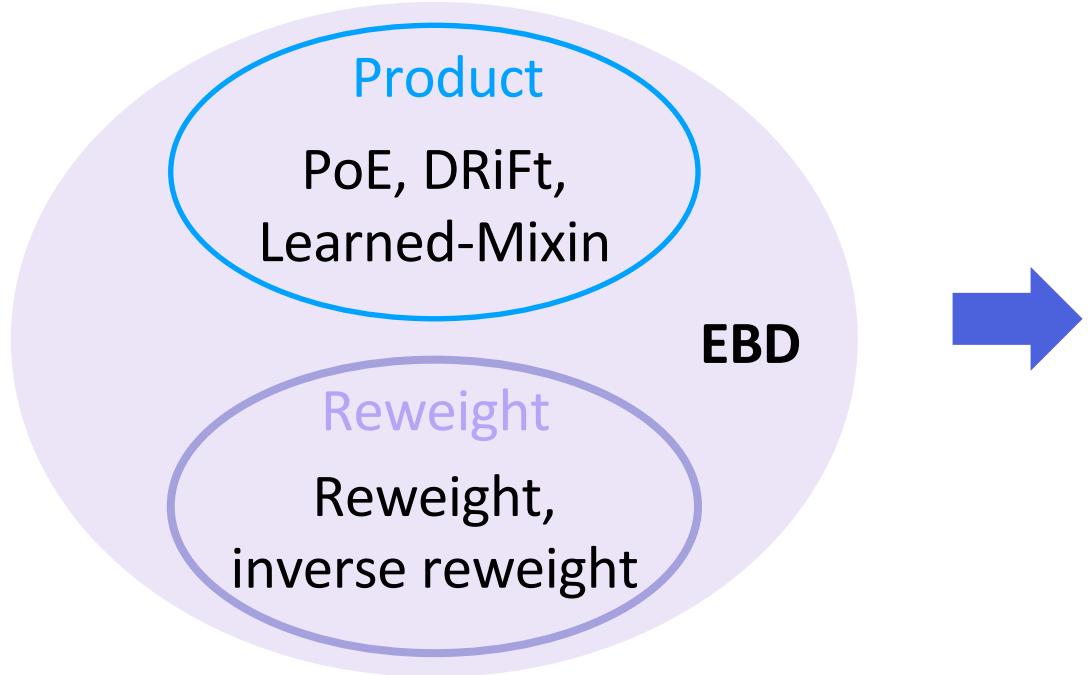
- Product methods $\min_{f_M} \mathbb{E}_{X,Y \sim \mathbb{P}_{\mathcal{D}}} [\mathcal{L}_c(Y, m(\mathbf{q}^b(X) \cdot \mathbf{q}^m(X)))]$,
 - Product-of-Experts: probability output
 - DRIFT: exponential of the logits output
- Re-weight methods $\min_{f_M} \mathbb{E}_{X,Y \sim \mathbb{P}_{\mathcal{D}}} \left[\frac{1}{p_Y^b(X)} \mathcal{L}_c(Y, \mathbf{p}^m(X)) \right]$,
 - Inverse reweight: probability output

Previous work focus on training unbiased model given bias-only model

Contents

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 - Why calibration?
- Method and Experiments
- Conclusion and Future Work

Ensemble Strategies



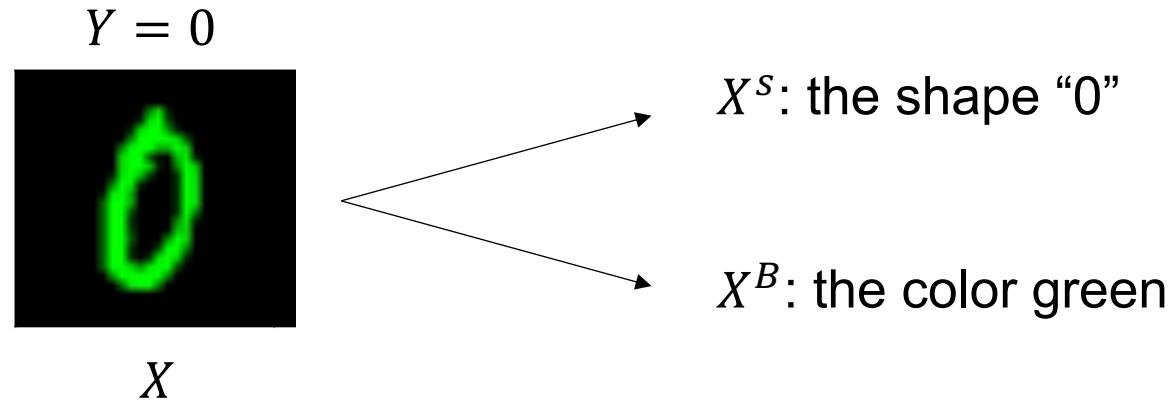
$$p^{m*} \propto \frac{\mathbb{P}_{\mathcal{D}}(Y | X)}{p^b}$$

the uncertainty estimation
of the bias-only model

The best main model relies on the uncertainty estimation of the bias-only model !

Theoretical Basis of EBD

- The signal and bias



$$\mathbb{P}_{\mathcal{D}}(Y|X^S) = \mathbb{P}_{\mathcal{D}'}(Y|X^S), \forall \mathcal{D}, \mathcal{D}' \quad \text{The intrinsic (invariant) principle}$$

$\mathbb{P}_{\mathcal{D}}(Y|X^B)$ usually **changes** across different \mathcal{D}

Theoretical Basis of EBD

- **The decomposition**

$$\mathbb{P}_{\mathcal{D}}(Y \mid X = x) \propto \mathbb{P}_{\mathcal{D}}(Y \mid X^B = x^b) \mathbb{P}_{\mathcal{D}}(Y \mid X^S = x^s) \frac{1}{\mathbb{P}_{\mathcal{D}}(Y)}$$

E.g. Conditional independence $X^S \perp\!\!\!\perp X^B \mid Y$

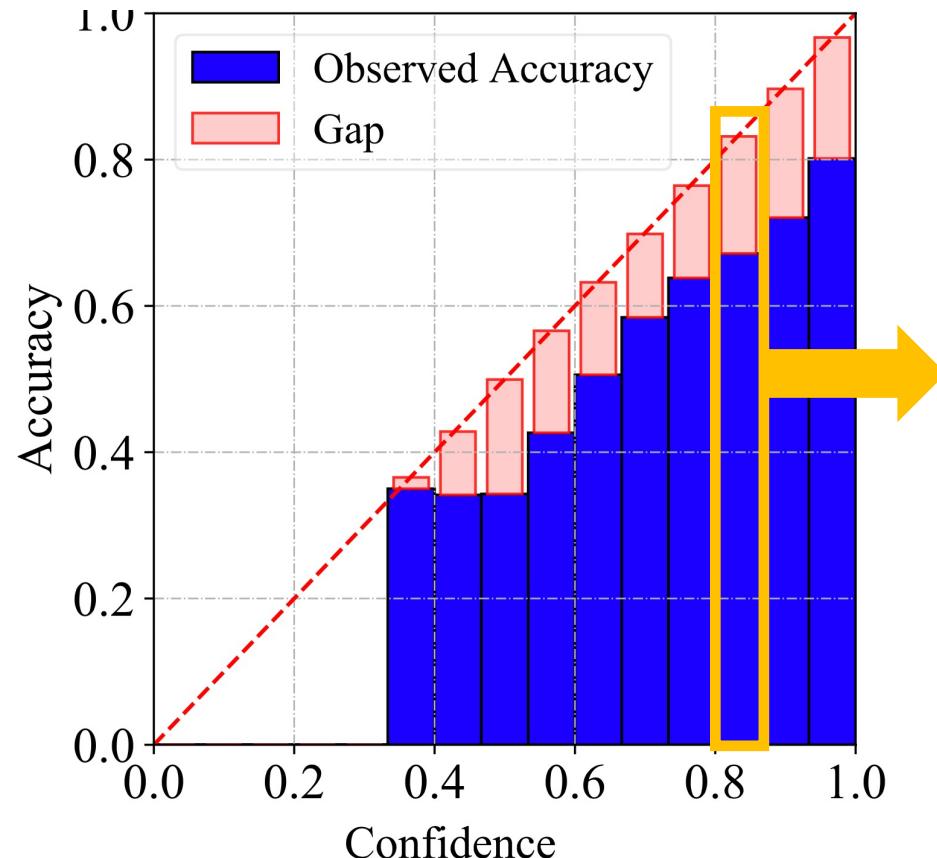
$$\mathbf{p}^{m*} \propto \frac{\mathbb{P}_{\mathcal{D}}(Y \mid X)}{\mathbf{p}^b}$$



When $\mathbf{p}^b \propto \mathbb{P}_{\mathcal{D}}(Y \mid X^B)$, $\mathbf{p}^{m*} \propto \mathbb{P}_{\mathcal{D}}(Y \mid X^S)$

The Calibration Problem

Modern machine learning models are poorly calibrated, many are overconfident (Guo et al. 2019)

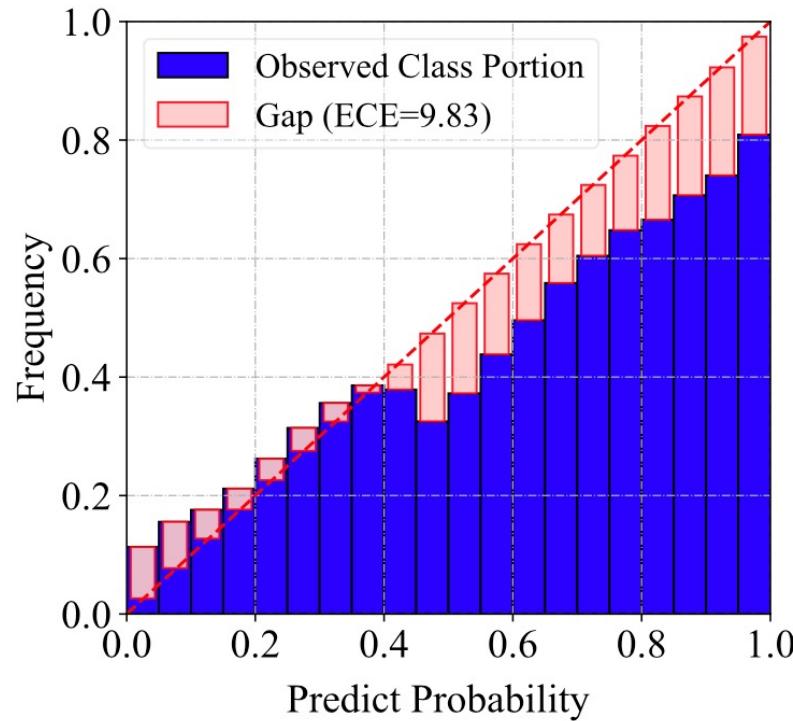


$$\mathbb{P}_{model}(\text{label} = i | x) \approx 0.85$$

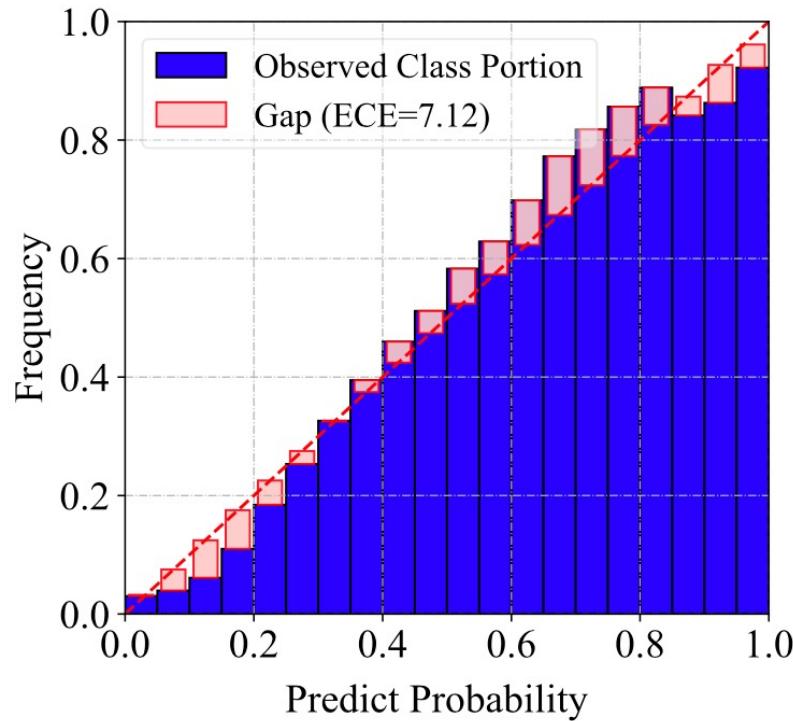
$$\mathbb{P}[\text{real label} = i | \mathbb{P}_{model}(\text{label} = i | x) \approx 0.85] \approx 0.65$$

The confidence of model is higher than its accuracy!
----- “over confident”(otherwise, lower)

Evidence: Poorly Calibrated Bias-only Models



(a) MNLI



(b) FEVER

Bias-only models in EBD methods are poorly calibrated

The Importance of Calibration

- **Theorem 1 (debiasing performance)**

The out-of-distribution accuracy of the debiased model is **monotonically decreasing with the calibration error** of the bias-only model when such error exceeds a threshold

Theorem 1. For any $l \in [0, 1]$, assume that $\exists l_0$ s.t. $\mathbb{P}_{\mathcal{D}}(Y = 0|X^B) \in (l_0 - \epsilon, l_0 + \epsilon)$ when X takes values in $\mathcal{S}_{f_B}(l)$. If the calibration error $|l - \mathbb{P}_{\mathcal{D}}(Y = 0|\mathcal{S}_{f_B}(l))| \geq \delta(l_0, \epsilon, \alpha) > 0$, the debiasing performance $\mathbb{P}_{\mathcal{D}}(\{x \in \mathcal{S}_{f_B}(l)|\tilde{Y}(x) = Y(x)\})$ declines as $|l - \mathbb{P}_{\mathcal{D}}(Y = 0|\mathcal{S}_{f_B}(l))|$ increases, where $\delta(l_0, \epsilon, \alpha)$ is a constant dependent with l_0 , ϵ and α . When $\alpha < \frac{1}{2} + \frac{\epsilon}{2l_0(1-l_0)+2\epsilon^2}$, $0 \leq \delta(l_0, \epsilon, \alpha) < 2\epsilon$, where $2\epsilon \leq \frac{\epsilon}{2l_0(1-l_0)+2\epsilon^2} < \frac{1}{2}$. Otherwise $C < \delta(l_0, \epsilon, \alpha) < 2\epsilon + C$, where $0 < C := l_0 - \epsilon - \frac{l_0+\epsilon}{(l_0+\epsilon)+(1-l_0-\epsilon)\frac{\alpha}{1-\alpha}}$, which increases as α increases.

The Importance of Calibration

- **Theorem 2 (In distribution performance)**

Theorem 2. *For any X , $\tilde{Y}(X) \neq \hat{Y}(X)$ if and only if $p_{\hat{Y}(x)}^b(x) > \mathbb{P}_{\mathcal{D}}(Y = \hat{Y}(x)|X = x)$.*

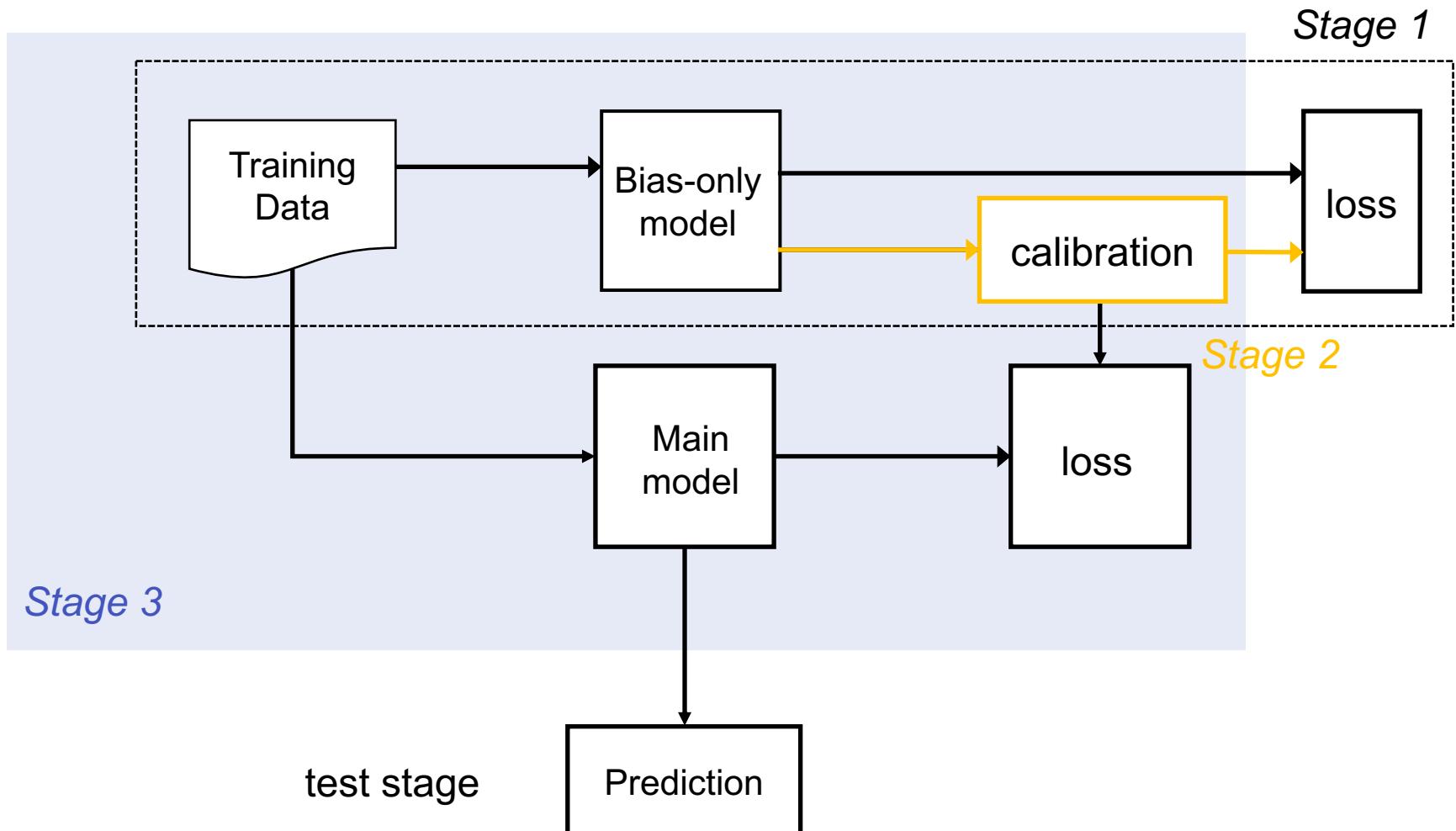
The in-distribution error is **non-decreasing** as the range of the uncertainty estimation of bias-only models increases

An important case: when the bias-only model is over-confident, decreasing its calibration error can **improve both the in-distribution and out-of-distribution** performance of the debiased model according to the two theorems

Contents

- Background
- Motivation
- Method and Experiments
 - 3 stage
 - Improvements and verification
- Conclusion and Future Work

Our Framework: MoCaD



Our Framework: MoCaD

- Temperature Scaling (Guo, 2017)

$$L = \frac{1}{n} \sum_{i=1}^n \text{logloss}(\sigma(\mathbf{z}/T), y_i)$$

- Dirichlet (Kull, 2019)  **Stronger**

$$\hat{\mu}_{\text{DirLin}}(\mathbf{q}; \mathbf{W}, \mathbf{b}) = \sigma(\mathbf{W} \ln \mathbf{q} + \mathbf{b})$$

$$L = \frac{1}{n} \sum_{i=1}^n \text{log los}(\hat{\mu}_{\text{DirLin}}(\hat{\mathbf{p}}(\mathbf{x}_i); \mathbf{W}, \mathbf{b}), y_i) + \lambda \cdot \left(\frac{1}{k(k-1)} \sum_{i \neq j} w_{ij}^2 \right) + \mu \cdot \left(\frac{1}{k} \sum_j b_j^2 \right)$$

Experiment: Datasets

| Task | Considered Bias | Train set | IID dev set | OOD test set |
|-------------------|-----------------|-----------|-------------|--------------------------------|
| NLI | Syntactic | MNLI | MNLI | HANS |
| | Hypothesis-only | | | MNLI-Hard-CD MNLI-Hard-SP |
| | Unknown | | | HANS |
| Fact Verification | Claim-only | FEVER | FEVER | FEVER-Symm v1 FEVER-Symm v2 |

Experiment: Metrics for Calibration

- Class-wise Expected Calibration Error (Class-wise ECE)

$$\text{classwise-ECE} = \frac{1}{k} \sum_{j=1}^k \sum_{i=1}^m \frac{|B_{i,j}|}{n} |y_j(B_{i,j}) - \hat{p}_j(B_{i,j})|$$



Difference between average prediction of class j probability
and the actual proportion of class j in the bin $B_{i,j}$

Experiment: Calibration Results

- Bias-only models after calibration ...

| | FEVER | HANS | MNLI | Unknown |
|-----------|-------|------|------|---------|
| Un-Cal | 7.11 | 9.83 | 3.01 | 7.41 |
| TempS | 6.23 | 7.70 | 2.38 | 3.07 |
| Dirichlet | 1.73 | 4.47 | 0.87 | 1.45 |



Classwise-ECE used to measure the performance of calibration, the lower the better

Classwise-ECE significantly drops on all datasets illustrate the effect of TempS & Dirichlet

Experiment: Results on FEVER

| Method | In-distribution | Test (out-of-distribution) | |
|----------------------------------|-----------------|----------------------------------|----------------------------------|
| | ID | Symm. v1 | Symm. v2 |
| CE | 87.1 ± 0.6 | 56.5 ± 0.9 | 63.9 ± 0.9 |
| PoE | 84.0 ± 1.0 | 62.0 ± 1.3 | 65.9 ± 0.6 |
| PoE_{TempS} | 82.0 ± 0.9 | 63.3 ± 0.9 | 66.4 ± 0.8 |
| PoE_{Dirichlet} | 87.1 ± 1.0 | 65.9 ± 1.1 | 69.1 ± 0.8 |
| DRiFt | 84.2 ± 1.2 | 62.3 ± 1.5 | 65.9 ± 0.7 |
| DRiFt_{TempS} | 81.7 ± 0.9 | 63.5 ± 1.3 | 66.5 ± 0.7 |
| DRiFt_{Dirichlet} | 87.4 ± 1.2 | 65.7 ± 1.4 | 69.0 ± 1.3 |
| InvR | 84.3 ± 0.8 | 60.8 ± 1.2 | 65.2 ± 1.0 |
| InvR_{TempS} | 83.8 ± 0.6 | 61.5 ± 0.9 | 65.4 ± 0.7 |
| InvR_{Dirichlet} | 87.0 ± 0.8 | 63.8 ± 2.2 | 68.2 ± 1.7 |
| LMin | 84.7 ± 1.8 | 59.8 ± 2.7 | 65.3 ± 1.1 |
| LMin_{TempS} | 84.9 ± 1.7 | 60.0 ± 2.5 | 65.6 ± 1.5 |
| LMin_{Dirichlet} | 87.5 ± 1.1 | 61.5 ± 2.4 | 67.1 ± 1.3 |



Consistently better performance in OOD and Dirichlet is a better one

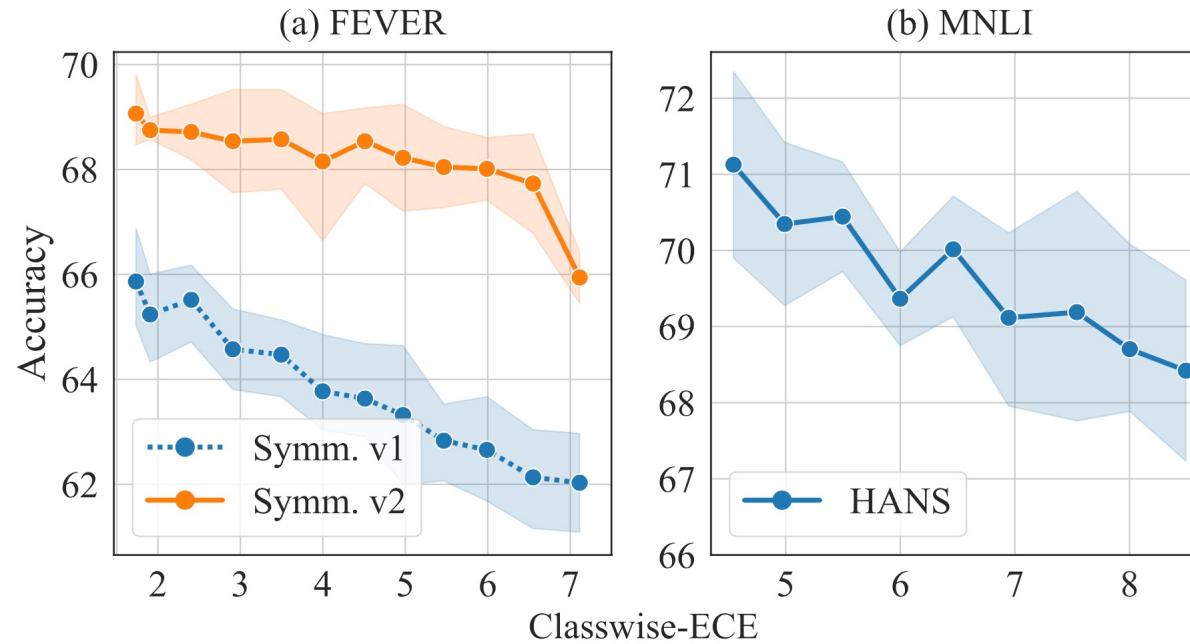
Experiment: Results on MNLI-HANS/MNLI-Hard

| Method | Test (out-of-distribution) | | | | | | | |
|----------------------------------|----------------------------|-------------------|----------------------|--------------------|--------------------|--------------|-------------------|--|
| | Syntactic Bias | | Hypothesis-only Bias | | | Unknown Bias | | |
| | ID | HANS | ID | Hard _{CD} | Hard _{SP} | ID | HANS | |
| CE | 84.2 ± 0.2 | 61.2 ± 3.2 | 84.2 ± 0.2 | 76.8 ± 0.4 | 72.6 ± 2.0 | 84.2 ± 0.2 | 61.2 ± 3.2 | |
| PoE | 82.8 ± 0.4 | 68.1 ± 3.4 | 83.2 ± 0.2 | 79.4 ± 0.4 | 76.8 ± 2.4 | 80.7 ± 0.2 | 69.0 ± 2.4 | |
| PoE_{TempS} | 83.9 ± 0.3 | 69.1 ± 2.8 | 82.9 ± 0.3 | 79.6 ± 0.4 | 77.4 ± 2.4 | 82.1 ± 0.2 | 69.9 ± 1.6 | |
| PoE_{Dirichlet} | 84.1 ± 0.3 | 70.7 ± 1.5 | 82.7 ± 0.4 | 79.4 ± 0.2 | 77.6 ± 2.1 | 82.3 ± 0.3 | 70.7 ± 1.0 | |
| DRiFt | 81.8 ± 0.4 | 66.5 ± 4.0 | 83.5 ± 0.4 | 79.5 ± 0.6 | 76.3 ± 1.6 | 80.2 ± 0.3 | 69.1 ± 1.3 | |
| DRiFt_{TempS} | 83.0 ± 0.4 | 69.7 ± 1.8 | 83.1 ± 0.2 | 79.6 ± 0.2 | 77.4 ± 3.3 | 81.5 ± 0.3 | 70.0 ± 0.9 | |
| DRiFt_{Dirichlet} | 83.6 ± 0.3 | 69.8 ± 1.9 | 82.8 ± 0.3 | 79.6 ± 0.2 | 79.0 ± 1.6 | 81.9 ± 0.6 | 69.4 ± 1.1 | |
| InvR | 82.5 ± 0.1 | 68.4 ± 1.2 | 83.1 ± 0.2 | 78.4 ± 0.5 | 77.1 ± 2.0 | 78.7 ± 4.8 | 64.7 ± 2.6 | |
| InvR_{TempS} | 83.6 ± 0.2 | 69.4 ± 1.6 | 82.8 ± 0.2 | 78.6 ± 0.2 | 77.9 ± 1.7 | 81.4 ± 0.5 | 65.8 ± 0.9 | |
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| LMin | 84.1 ± 0.3 | 65.5 ± 3.7 | 80.5 ± 0.3 | 80.0 ± 0.4 | 78.2 ± 2.0 | 83.1 ± 0.3 | 66.5 ± 1.1 | |
| LMin_{TempS} | 84.1 ± 0.2 | 63.2 ± 2.7 | 80.5 ± 0.6 | 80.3 ± 0.2 | 80.8 ± 3.6 | 83.3 ± 0.2 | 66.2 ± 1.0 | |
| LMin_{Dirichlet} | 84.3 ± 0.3 | 62.7 ± 2.6 | 80.1 ± 0.5 | 79.8 ± 0.4 | 83.2 ± 2.2 | 82.7 ± 0.2 | 66.4 ± 1.2 | |



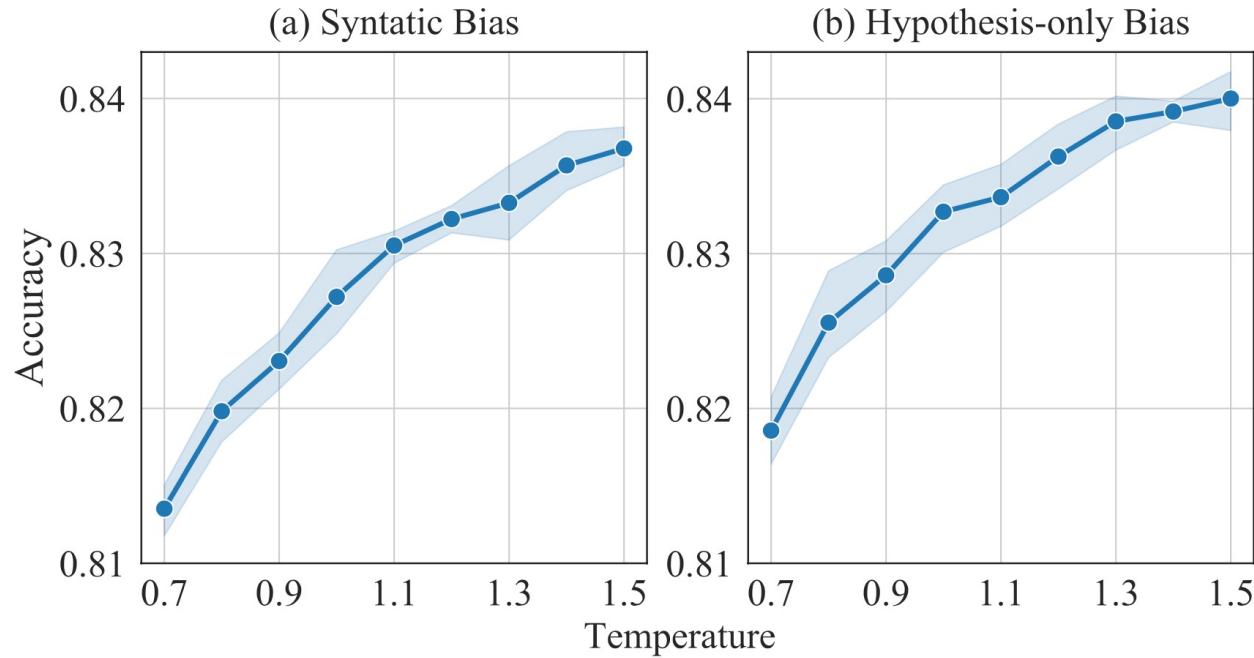
Consistently better performance in OOD and Dirichlet is a better one

Empirical Verification of Theorem 1 (On debiasing performance)



Debiasing performance of bias-only model decreases as the classwise-ECE goes up

Empirical Verification of Theorem 2 (On IID performance)



Bigger temperature -> lower confidence -> better in-distribution performance

Empirical Verification: Over/under Confident

| Method | Syntactic Bias | | Hypothesis-only Bias | | | Unknown Bias | |
|--------------------------|----------------|----------------|----------------------|--------------------|--------------------|----------------|----------------|
| | ID | HANS | ID | Hard _{CD} | Hard _{SP} | ID | HANS |
| CE | 84.2 ± 0.2 | 61.2 ± 3.2 | 84.2 ± 0.2 | 76.8 ± 0.4 | 72.6 ± 2.0 | 84.2 ± 0.2 | 61.2 ± 3.2 |
| PoE | 82.8 ± 0.4 | 68.1 ± 3.4 | 83.2 ± 0.2 | 79.4 ± 0.4 | 76.8 ± 2.4 | 80.7 ± 0.2 | 69.0 ± 2.4 |
| PoE _{TempS} | 83.9 ± 0.3 | 69.1 ± 2.8 | 82.9 ± 0.3 | 79.6 ± 0.4 | 77.4 ± 2.4 | 82.1 ± 0.2 | 69.9 ± 1.6 |
| PoE _{Dirichlet} | 84.1 ± 0.3 | 70.7 ± 1.5 | 82.7 ± 0.4 | 79.4 ± 0.2 | 77.6 ± 2.1 | 82.3 ± 0.3 | 70.7 ± 1.0 |

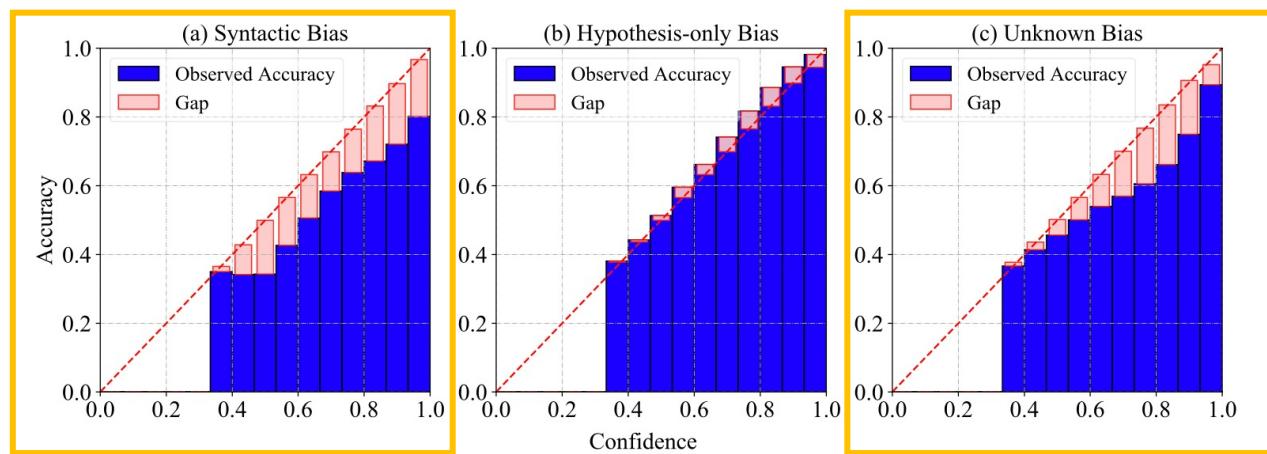


Figure 1: Reliability diagrams of the bias-only models on MNLI. On MNLI, (a) the syntactic bias-only model and (c) the unknown bias-only model are over-confident, (b) the hypothesis-only bias-only model is under-confident.

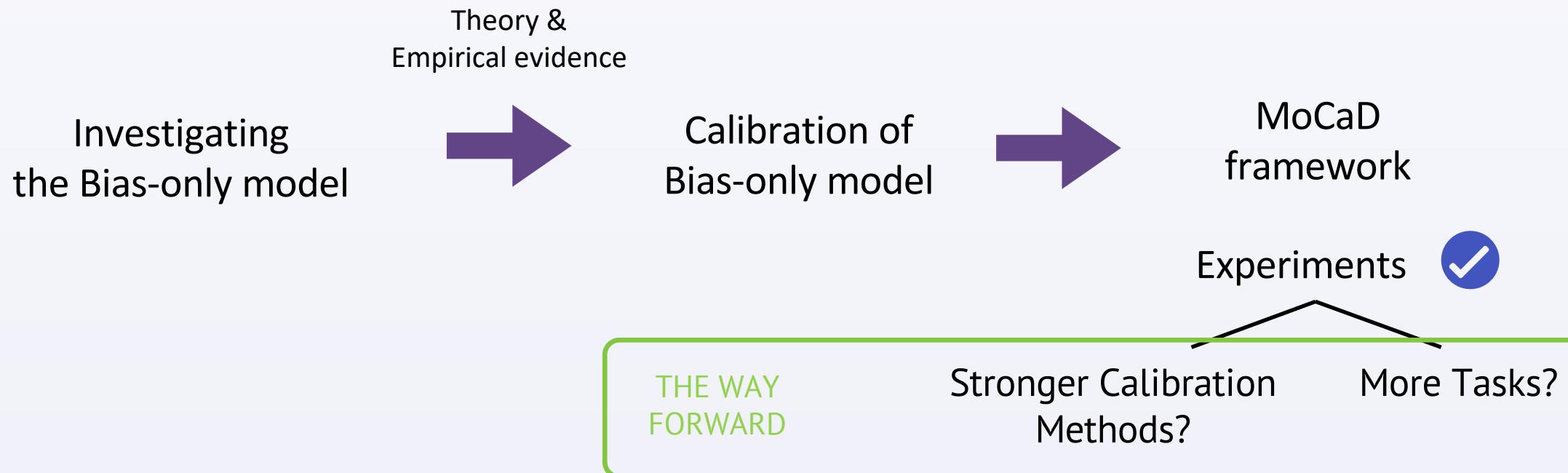
Calibration of over-confident bias-only benefits performance on both in and out of distribution

Contents

- Background
- Motivation
- Method and Experiments
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Uncertainty Calibration for Ensemble-Based Debiasing Methods

Ruixin Xiong*, Yimeng Chen*, Liang Pang, Xueqi Cheng, Zhiming Ma, Yanyan Lan



Experiments on Image Classification

Table 2: Classification accuracy on image classification.

| Method | ID | UnBiased | ImageNet-A |
|----------------------------------|----------------|----------------------------------|----------------------------------|
| PoE | 94.6 ± 0.2 | 94.3 ± 0.3 | 31.8 ± 1.9 |
| PoE_{TempS} | 94.7 ± 0.3 | 94.5 ± 0.3 | 31.9 ± 1.1 |
| PoE_{Dirichlet} | 94.6 ± 0.4 | 94.3 ± 0.4 | 30.5 ± 1.2 |
| DRiFt | 94.6 ± 0.2 | 94.4 ± 0.3 | 31.9 ± 0.8 |
| DRiFt_{TempS} | 94.8 ± 0.4 | 94.4 ± 0.4 | 32.5 ± 1.2 |
| DRiFt_{Dirichlet} | 94.5 ± 0.2 | 94.3 ± 0.2 | 32.4 ± 1.0 |
| InvR | 94.5 ± 0.4 | 94.1 ± 0.5 | 31.6 ± 0.3 |
| InvR_{TempS} | 94.3 ± 0.1 | 93.8 ± 0.1 | 32.2 ± 1.5 |
| InvR_{Dirichlet} | 94.4 ± 0.4 | 94.2 ± 0.2 | 31.8 ± 0.9 |
| LMin | 90.9 ± 0.5 | 90.5 ± 0.6 | 27.7 ± 1.6 |
| LMin_{TempS} | 91.1 ± 0.6 | 90.6 ± 0.6 | 28.1 ± 1.8 |
| LMin_{Dirichlet} | 91.2 ± 0.2 | 90.9 ± 0.2 | 26.1 ± 0.8 |

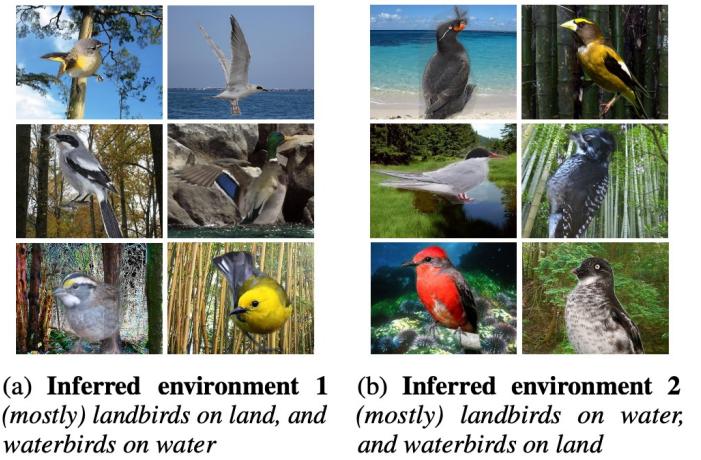
Experiments on 9-Class ImageNet dataset

MoCaD can achieve the best debiasing performance among all EBD methods, but the improvement is inconsistent.

In Progress: Invariant learning for Debiasing

- Invariant learning for debiasing:
 - Infer environments
 - Minimize the loss with an invariance penalty

$$\min_{f,\theta} \sum_{e \in \mathcal{E}} \lambda_e \mathcal{R}^e(f, \theta) + \lambda \cdot \text{penalty}(\{S_e(f, \theta)\}_{e \in \mathcal{E}})$$



- Problem:
 - Optimal solution of Invariant learning may still rely on bias
 - Unstable performance
- Our contribution:
 - Prove necessary and sufficient conditions for the equivalence of invariant learning and debiasing
 - Propose a new method based on the theory



Thanks for Your Attention !