Direct Confidence Alignment: Aligning Verbalized Confidence with Internal Confidence In Large Language Models

Anonymous ACL submission

Abstract

Producing trustworthy and reliable Large Language Models (LLMs) has become increasingly important as their usage becomes more widespread. Calibration seeks to achieve this by improving the alignment between the model's confidence and the actual likelihood of its responses being correct or desirable. However, it has been observed that the internal confidence of a model, derived from token probabilities, is not well aligned with its verbalized confidence, leading to misleading results with different calibration methods. In this paper, we propose Direct Confidence Alignment (DCA), a method using Direct Preference Optimization to align an LLM's verbalized confidence with its internal confidence rather than ground-truth accuracy, enhancing model transparency and reliability by ensuring closer alignment between the two confidence measures. We evaluate DCA across multiple open-weight LLMs on a wide range of datasets. To further assess this alignment, we also introduce three new calibration error-based metrics. Our results show that DCA improves alignment metrics on certain model architectures, reducing inconsistencies in a model's confidence expression. However, we also show that it can be ineffective on others, highlighting the need for more model-aware approaches in the pursuit of more interpretable and trustworthy LLMs.

1 Introduction

LLMs have revolutionized natural language tasks, achieving impressive performance across various applications (Wei et al., 2022; Naveed et al., 2024) Despite their capabilities, there are still concerns about the calibrations of these models, that is, the alignment between the confidence they assign to their predictions and the actual accuracy of those predictions(Jiang et al., 2021). For example, in a well-calibrated model, predictions assigned a 70% confidence level should be correct approximately 70% of the time. These limitations are especially critical in high-risk applications such as decision support systems, healthcare settings (Peng et al., 2023), and legal consultations (Lai et al., 2024), where overconfidence in incorrect answers can lead to severe consequences. Examples include erroneous recommendations in decision support systems that can lead to significant financial operational losses, misdiagnoses in healthcare, and flawed legal advice that may affect case outcomes.

Existing model confidence estimation methods can be categorized into two types: Internal and Verbalized Confidence.

Internal Confidence (C_i) is most commonly quantified as the probability of predicting a particular output token semantically linked to an answer given a context. There have also been alternative approaches to estimating internal confidence, such as self-consistency-based approaches and ensemble methods (Geng et al., 2024; Portillo Wightman et al., 2023).

Verbalized Confidence (C_v) is defined as the LLM's expression of its confidence level as a certainty percentage in its output answer to a given prompt (Lin et al., 2022a).

Whilst existing literature predominantly focuses on accuracy-based calibration, which involves aligning models' predicted confidence with ground-truth accuracy, they do not cover the effects of calibrating verbalized confidence C_v to internal confidence C_i instead of against accuracy. Furthermore, internal confidence C_i derived from logits and verbalized confidence within LLMs are often misaligned with each other, leading to inconsistent confidence expressions, especially in unfamiliar questions where models can be verbally overconfident (Ni et al., 2024).

To address these, we propose Direct Confidence Alignment: a method that involves aligning verbalized confidence C_v with internal confidence C_i using DPO (Rafailov et al., 2024). By aligning verbalized confidence with internal confidence, we

argue that models can provide a more transparent and consistent view of their confidence in their responses. We evaluate our approach on a range of datasets and alignment metrics. We make the following contributions:

1. We introduce a novel method of aligning verbalized confidence C_v with internal confidence C_i using DPO training, taking internal confidence as ground truth to improve the transparency and reliability of LLMs.

2. We show the effects and implications of DCA on various LLMs with a wide range of architectures across multiple datasets, highlighting its varied impact across models.

3. We introduce and evaluate our method on three new metrics based on calibration error, which in this paper refers to the model's internal confidence C_i subtracted from its verbalized confidence C_v for each response. Our proposed metrics in 4.3 provide a more detailed assessment of the magnitude and consistency of alignment between verbalized and internal confidence within LLMs.

2 Related Works

Confidence Calibration Calibration has been an area of extensive research in LLMs. (Lin et al., 2022a; Park and Caragea, 2022; Kadavath et al., 2022; Kuhn et al., 2022; Guo et al., 2017) show that a pre-trained LLM's calibration can improve with model size, fine-tuning, prompting, self-consistency, or post-hoc methods such as temperature scaling. Temperature scaling in LLM calibration applies a single scalar parameter to adjust model logits before softmax. Known for its simplicity and effectiveness in improving calibration while preserving accuracy, it outperforms techniques such as Platt scaling and isotonic regression across a range of NLP tasks (Guo et al., 2017; Desai and Durrett, 2020). Other approaches involve forms of self-consistency, however, (Zhao et al., 2021) demonstrate that a model's confidence can be sensitive to prompting variation. To address this, (Wang et al., 2024; Portillo Wightman et al., 2023) generates an ensemble of prompts, using prompt agreement to generate a calibrated confidence. More recently, (Tao et al., 2024) proposes Confidence-Quality-Order-preserving alignment approach, which incentivizes the model to verbalize greater confidence for responses of higher quality, addressing the lack of a definite ground truth standard for confidence that aligns with response quality in other methods.

Verbalized Confidence As model logits are either inaccessible in black box LLMs or rendered inaccurate due to RLHF, recent work (Tian et al., 2023; Xiong et al., 2024) explores the calibration of verbalized confidence. For example, (Tian et al., 2023) takes the mean of k verbalized confidence samples; however, it is sensitive to the prompting structure, making it difficult to generalize sequential reasoning and limited to short answers. To explore this, (Xiong et al., 2024) asks the model to elicit verbal confidences using different temperatures and prompt strategies, including Chain-of-Thought, Multi-Step, and Top-K reasoning.

Unlike the above techniques for confidence calibration, our work seeks to align a model's verbalized confidence with its internal confidence, making no reference to ground-truth accuracy or response quality.

Confidence-Probability Alignment (Kumar et al., 2024) introduces the concept of Confidence-Probability Alignment, a measurement of the correlation between a model's verbalized certainty and its internal confidence, quantified using answer token probabilities. They posit that Confidence-Probability Alignment is crucial for the reliability of a model's output. Our work expands on this study by aligning these two confidence measures using DPO.

Direct Preference Optimization (Rafailov et al., 2024) demonstrates that Direct Preference Optimization (DPO) achieves comparable or superior performance to existing reinforcement learning from human feedback (RLHF) methods in various text generation tasks while being computationally efficient. Although they show that DPO has previously been successfully used to align LLMs with human preferences in sentiment control and improve dialogue quality, our work focuses on the fact that DPO uses a preference dataset to serve as a learning signal for preferred and non-preferred model outputs as opposed to a reward function, making it ideal for aligning a model's verbalized confidence with its internal confidence in a pairwise format.

3 Methodology

We define DCA as a method to improve the alignment between verbalized confidence and internal confidence within LLMs using DPO, expanding on the study of (Kumar et al., 2024), which introduced this concept.

3.1 Verbalized Confidence Extraction

To extract the model's verbalized confidence C_v, we prompt it in the format of our prompt template in A.1 and extract the C_v from its output.

3.2 Internal Confidence Extraction

To extract the model's internal confidence C_i, we use the computed probability of the answer token (e.g., A, B, C, D) in its output.

3.3 Preference Dataset Creation

To generate an entry in our preference dataset for DPO training, we first generate a sample with full-text completion via our base prompt in A.1 to obtain a formatted answer. We then extract C_i using our method in 3.2 and extract C_v from the model response. Using these values, we create two versions of the answer:

Original Response: Original response of the model
Modified Response: A copy of the original response where the model's C_v is overwritten with its C_i.

For each entry in our preference dataset, the modified response will be the chosen option, and the original response will be the rejected option. See Figure 1 for a visual summary of this process.

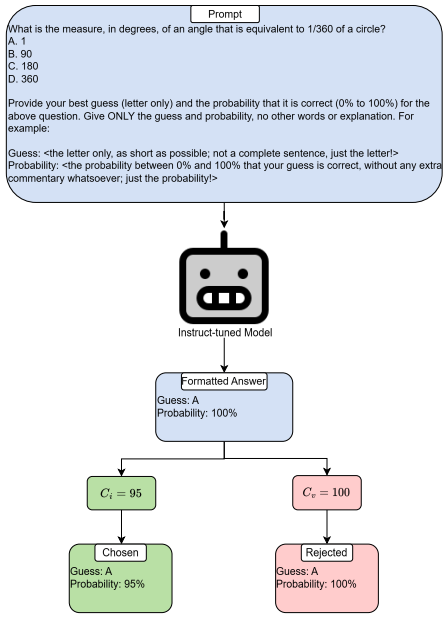

Figure 1: An overview of the entry generation process for our preference dataset. Sample question and response are from MMLU elementary mathematics and Gemma 2-9B-Instruct, respectively.

4 Experiment

4.1 Models

We use three open-weight instruct tuned LMs for our experimental setup, namely Meta's Llama 3.2-3B-Instruct (Team, 2024b); Google's Gemma 2-9B-Instruct (Team, 2024a); and Mistral AI's Mistral 7B-Instruct (Team, 2023).

4.2 Datasets

We use the following datasets for experimentation:

- *OpenBookQA* (Mihaylov et al., 2018) - A science multiple choice dataset modelled after open-book exams testing knowledge and applications of facts
- *TruthfulQA* (Lin et al., 2022b) - A dataset crafted to test LLMs' ability to truthfully answer questions. Scoring well reflects the model's ability to avoid generating false answers from imitating human text.
- *CosmosQA* (Huang et al., 2019) - A reading comprehension dataset based on common sense and reading between the lines for a diverse set of personal everyday narratives.
- *Massive Multitask Language Understanding* (MMLU) (Hendrycks et al., 2021) - An evaluation benchmark designed to test knowledge gained from pretraining, containing 57 subjects and a wide range of difficulty levels.

For the preference dataset, we use samples from the "train" split of CosmosQA and an equal number of samples split evenly between subjects in the "test" split of MMLU.

Model	Method	OpenBookQA				TruthfulQA				CosmosQA				MMLU				Mean			
		$\rho\uparrow$	$\sigma_\epsilon\downarrow$	$\overline{\lvert\epsilon\rvert}\downarrow$	$\sigma_M\downarrow$	$\rho\uparrow$	$\sigma_\epsilon\downarrow$	$\overline{\lvert\epsilon\rvert}\downarrow$	$\sigma_M\downarrow$	$\rho\uparrow$	$\sigma_\epsilon\downarrow$	$\overline{\lvert\epsilon\rvert}\downarrow$	$\sigma_M\downarrow$	$\rho\uparrow$	$\sigma_\epsilon\downarrow$	$\overline{\lvert\epsilon\rvert}\downarrow$	$\sigma_M\downarrow$	$\rho\uparrow$	$\sigma_\epsilon\downarrow$	$\overline{\lvert\epsilon\rvert}\downarrow$	$\sigma_M\downarrow$
Mistral-7B-Instruct	Vanilla	**0.17**	25.06	**20.08**	1.12	**0.20**	30.64	**25.99**	1.07	**0.20**	**20.59**	**19.53**	**0.53**	**0.18**	26.24	**24.25**	0.67	**0.19**	25.63	**22.96**	0.85
	DCA	0.14	**20.77**	47.83	**0.93**	0.06	**24.47**	43.90	**0.86**	0.16	23.23	52.47	0.59	0.17	**23.23**	51.53	**0.59**	0.13	**22.93**	48.93	**0.74**
Gemma-2-9B-Instruct	Vanilla	0.32	19.43	9.86	0.87	0.41	17.21	10.74	0.60	0.30	14.88	9.39	0.39	0.33	16.36	9.64	0.43	0.34	16.97	9.91	0.57
	DCA	**0.39**	**16.83**	**5.06**	**0.76**	**0.51**	**12.71**	**5.06**	**0.46**	**0.38**	**9.97**	**4.00**	**0.25**	**0.39**	**13.64**	**6.00**	**0.35**	**0.42**	**13.79**	**5.03**	**0.46**
Llama-3-2.3B-Instruct	Vanilla	**0.31**	42.01	**37.55**	1.90	**0.17**	43.40	38.48	1.57	**0.46**	37.91	**38.69**	0.97	0.18	43.45	**39.95**	1.15	**0.28**	41.19	**38.67**	1.40
	DCA	0.30	**23.20**	46.00	**1.04**	0.15	**23.76**	**38.04**	**0.83**	0.24	**21.00**	50.47	**0.54**	**0.22**	**23.54**	43.62	**0.60**	0.23	**22.88**	44.03	**0.75**

Table 1: Alignment evaluation across OpenBookQA, TruthfulQA, CosmosQA, and MMLU. ↑ indicates higher is better, ↓ indicates lower is better. Best values per column are bolded. Mean values of each metric for each model are also shown for aggregation. All values of ρ are significant (p < 0.01).

For the evaluation dataset, we use all questions from the "test" split of OpenBookQA and the "validation" split of TruthfulQA's multiple choice subset for evaluation on out-of-distribution (OOD) datasets, as well as an equal sample of questions from the "validation" splits of MMLU and CosmosQA for evaluation on in-distribution (ID) datasets.

4.3 Metrics

We use **Spearman's Rank Correlation Coefficient** ρ (Spearman.,1904) to directly evaluate the effectiveness of our method on improving Confidence-Probability Alignment (Kumar et al., 2024). However, ρ only measures the strength of a monotonic correlation and does not reference the perfect calibration line of $y = x$. Hence, we introduce and use **Standard Deviation of Calibration Error** σ_ϵ, **Mean Absolute Calibration Error** $\overline{|\epsilon|}$, and **Standard Error of Calibration Error** σ_M, as they can intrinsically reference the perfect calibration line of y=x as a global extremum and isolate the overall bias within the C_v of the models.

5 Results and Analysis

Table 1 presents our results for all models across all datasets. Gemma 2-9B-Instruct showed the strongest and most consistent improvements in metrics after DCA, demonstrating superior alignment across all datasets. Most notably, it demonstrated the largest improvements in ρ and $\overline{|\epsilon|}$ of all models on TruthfulQA. In contrast, mixed results were observed for Llama-3.2-3B-Instruct and Mistral-7B-Instruct across all datasets. For example, Llama-3.2-3B- Instruct demonstrates an increase in ρ from 0.18 to 0.22 for MMLU however ρ fell from 0.46 to 0.24 on CosmosQA. Mistral-7B-Instruct demonstrates a large increase in $\overline{|\epsilon|}$ from 19.53 to 52.47 for CosmosQA and a large reduction in ρ from 0.20 to 0.06 on TruthfulQA. These findings indicate that DCA is ineffective for these models on certain tasks. Gemma 2-9B-Instruct's consistent performance on OOD datasets suggest that DCA was effective at generalising its stronger alignment between C_v and C_i to unseen questions. σ_ϵ and σ_M improved across most models and datasets, suggesting that DCA lowered the variance in calibration error for all models, especially for Llama-3.2-3B-Instruct (see Figure 4 for an example). However, a low σ_ϵ is only useful if $\overline{|\epsilon|}$ is also low, which would indicate consistent and strong alignment between verbalized and internal confidence as shown by Gemma 2-9B-Instruct (see Figure 3 for an example). The similarity between results on ID datasets and OOD datasets across models also suggest that the effectiveness of DCA may be more model-dependent than task-dependent, relying more on the model architecture and how different models process confidence elicitation in QA tasks.

6 Conclusion

In this paper we present Direct Confidence Alignment: a method of using DPO to improve the alignment between verbalized and internal confidence in LLMs. Our results show that DCA can be effective at improving this alignment as demonstrated by Gemma 2-9B-Instruct, but also highlight the pressing need for improvements, such as expanding the method to be compatible with a wider range of model architectures and exploring more strategies to improve this alignment.

Limitations

Access to Logits This method is limited to models with access to internal logits to extract model internal confidence. This makes it inapplicable to state-of-the-art (SOTA) closed-source models.

Reliance on well calibrated token probabilities This method will be most useful if the internal con-

fidence of the model is better calibrated against accuracy than its verbalized confidence, and thus may require other ground-truth-based calibration techniques to be used in conjunction for best results.

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A Appendix

Model	OpenBookQA		TruthfulQA		CosmosQA		MMLU	
	Vanilla	DCA	Vanilla	DCA	Vanilla	DCA	Vanilla	DCA
Mistral-7B-Instruct	**59.00%**	58.23%	**32.84%**	20.98%	**60.48%**	54.02%	**55.91%**	48.85%
Gemma 2-9B-Instruct	86.06%	**86.21%**	59.68%	**60.85%**	79.63%	**80.01%**	**72.41%**	72.05%
Llama 3.2-3B-Instruct	47.14%	**64.00%**	29.71%	**37.75%**	66.43%	**73.55%**	39.92%	**49.77%**

Table 2: Comparison of accuracy across our datasets for models before and after DCA. Higher accuracy between Vanilla and DCA versions of each model are in bold.

A.1 Prompt Template

{Question}
{Options}

Provide your best guess (letter only) and the probability that it is correct (0% to 100%) for the above question. Give ONLY the guess and probability, no other words or explanation. For example:

Guess: <the letter only, as short as possible; not a complete sentence, just the letter!>
Probability: <the probability between 0% and 100% that your guess is correct, without any extra commentary whatsoever; just the probability!>

We use a slightly modified version of (Tian et al., 2023)'s Verb. 1S top-1 prompt as our prompt template. We match this prompt across all of our experiments and training processes to ensure consistent responses and output formats during training, and post-training evaluation.

A.2 DCA Training

For DPO training, we use the Unsloth library (Daniel Han and team, 2023) for improved training speeds and efficient memory usage. We loaded LoRA adapters onto our Instruct models using the configurations in Table 3 before training. Training was run on RTX 4000 Ada GPUs, and we used the `ipo` loss function (Azar et al., 2023) to avoid overfitting on the preference dataset. The complete training parameters can be found in Table 4.

A.3 Effects of DCA on accuracy

Table 2 shows that DCA can have mixed impacts on model accuracy. While accuracy remained stable on Gemma 2-9B-Instruct, Mistral-7B-Instruct demonstrated lower accuracies after DCA, especially on TruthfulQA. Interestingly, accuracy increased for Llama 3.2-3B-Instruct across all datasets.

A.4 Supplementary Figures

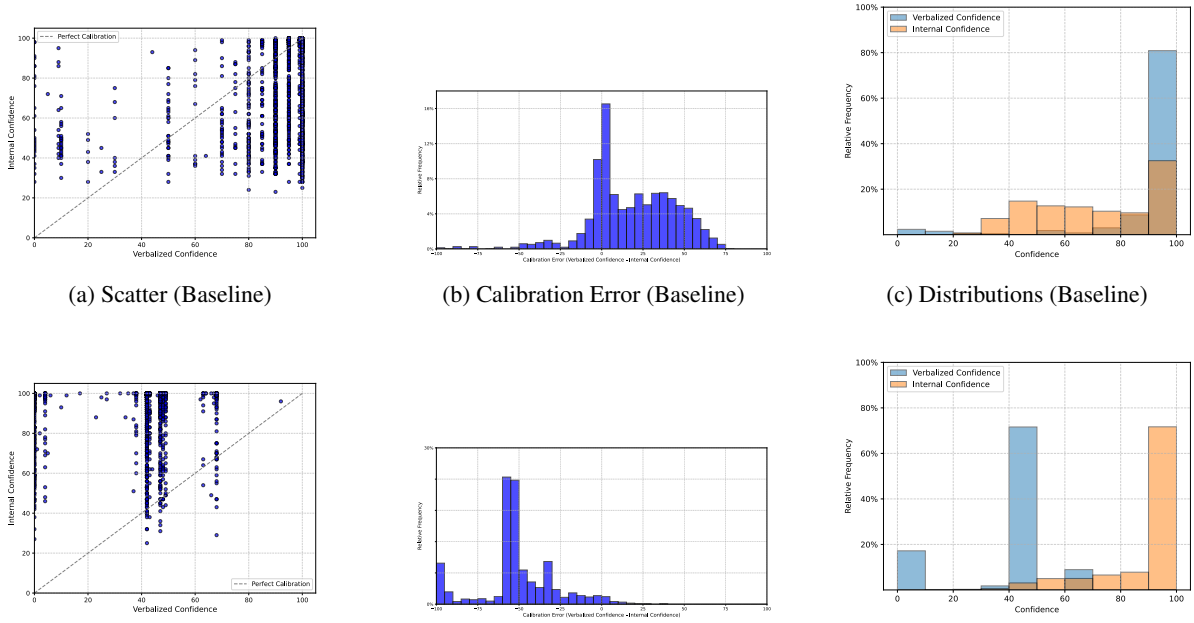
Figures 2,3,and 4 below show supplementary figures for the results of Mistral-7B-Instruct, Gemma 2-9B-Instruct, and Llama 3.2-3B-Instruct, respectively, along with their DCA-trained counterparts on MMLU. For each model, the observed visual trends were broadly consistent across the other datasets.

Hyperparameter	Value	Notes
r (LoRA rank)	16	Low-rank dimension for adapter updates
target_modules	`"q_proj"`, `"k_proj"`, `"v_proj"`, `"o_proj"`, `"gate_proj"`, `"up_proj"`, `"down_proj"`	Only these weight matrices receive LoRA updates
lora_alpha	16	Scales the low-rank updates
lora_dropout	0.0	No dropout on LoRA adapters
bias	`"none"`	Do not update any bias parameters in LoRA
`use_gradient_checkpointing`	`"unsloth"`	Unsloth's gradient-checkpointing strategy
random_state	3407	Seed for LoRA weight initialization and any randomness
use_rslora	False	Standard LoRA (RSLORA disabled)
loftq_config	None	No custom quantization configuration

Table 3: LoRA / PEFT Hyperparameters

Training Parameter	Value
logging_steps	10
loss_type	`ipo`
bf16	True
save_steps	100
`per_device_train_batch_size`	2
`gradient_accumulation_steps`	32
learning_rate (default)	1e-06
weight_decay (default)	0.0
num_train_epochs (default)	3
optimizer (default)	AdamW (β_1=0.9, β_2=0.999)
lr_scheduler_type (default)	constant (no warmup)
seed	3407

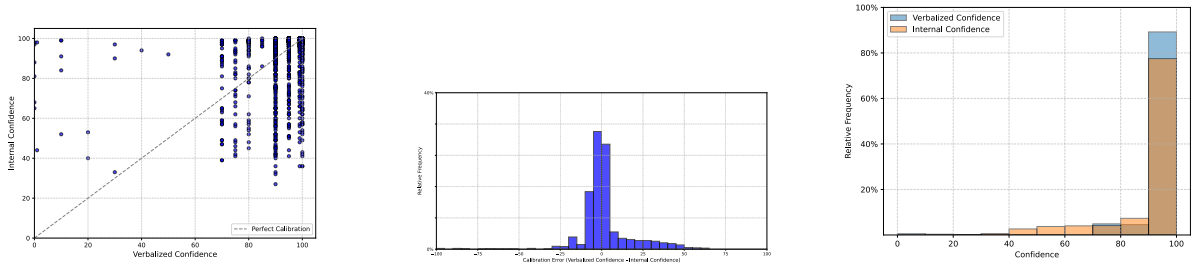
Table 4: DPO Fine-Tuning Hyperparameters



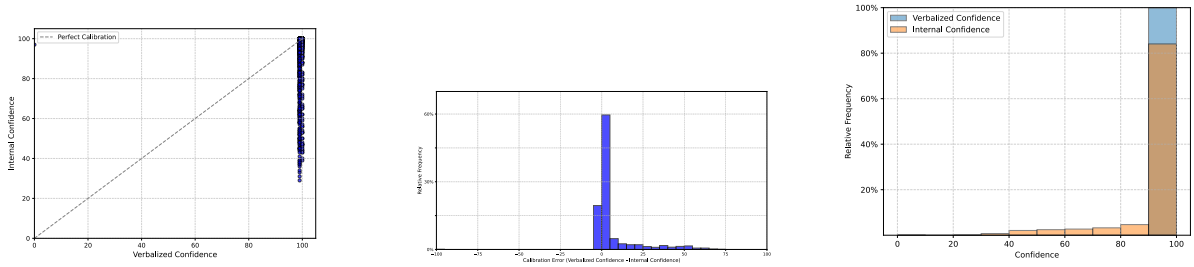
(a) Scatter (Baseline) (b) Calibration Error (Baseline) (c) Distributions (Baseline)

(d) Scatter (DCA) (e) Calibration Error (DCA) (f) Distributions (DCA)

Figure 2: Comparison of baseline vs. DCA-trained Mistral-7B-Instruct on MMLU. Top row: Verbalized vs. internal confidence scatter plot, calibration error histogram, and confidence score distributions for the baseline model. Bottom row: Same visualizations for the DCA-trained model.

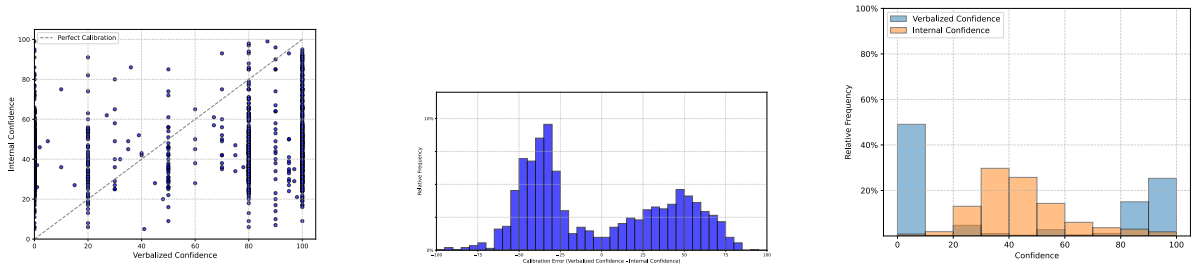


(a) Scatter (Baseline) (b) Calibration Error (Baseline) (c) Distributions (Baseline)

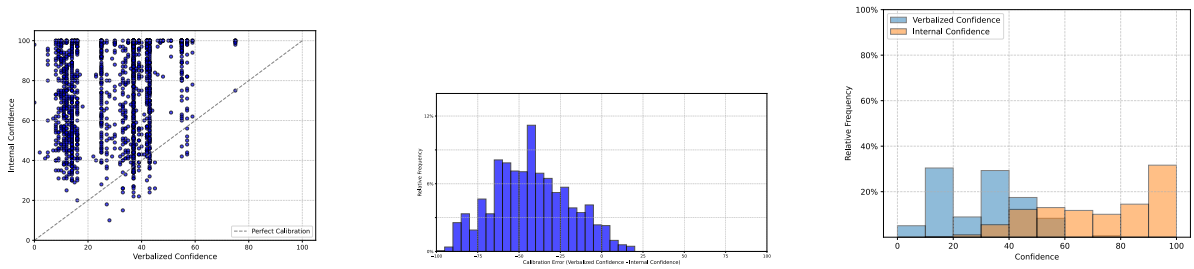


(d) Scatter (DCA) (e) Calibration Error (DCA) (f) Distributions (DCA)

Figure 3: Comparison of baseline vs. DCA-trained Gemma 2-9B-Instruct on MMLU. Top row: Verbalized vs. internal confidence scatter plot, calibration error histogram, and confidence score distributions for the baseline model. Bottom row: Same visualizations for the DCA-trained model.



(a) Scatter (Baseline) (b) Calibration Error (Baseline) (c) Distributions (Baseline)



(d) Scatter (DCA) (e) Calibration Error (DCA) (f) Distributions (DCA)

Figure 4: Comparison of baseline vs. DCA-trained Llama 3.2-3B-Instruct on MMLU. Top row: Verbalized vs. internal confidence scatter plot, calibration error histogram, and confidence score distributions for the baseline model. Bottom row: Same visualizations for the DCA-trained model.