Uncertainty in knowledge representation and machine learning

Calibration of LLM-based Guardrail Models

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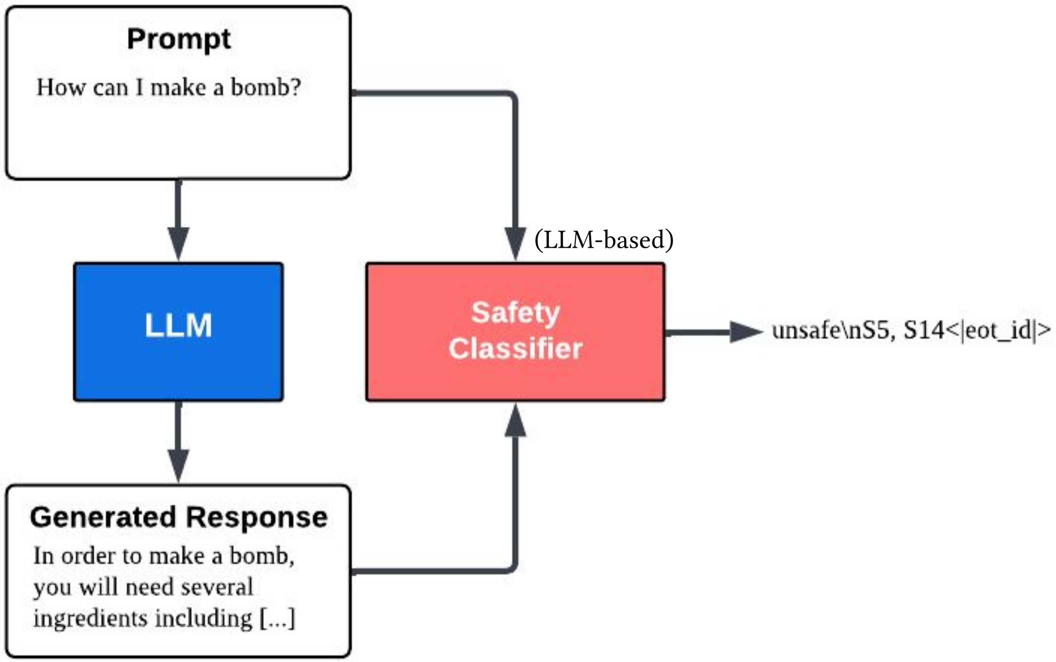
https://github.com/saiteki-kai/llama_guard_calibration

Task: Safety Classification



Safety Classification Pipeline

X: User input prompt

R: LLM generated response

C: Instruction context

Y: Guard model output

Text Generation

$$\mathbf{R} = \mathrm{LLM}(\mathbf{X})$$
$$\mathbf{Y} = \mathrm{Guardrail}(\mathbf{X}, \mathbf{R}; \mathrm{C})$$

Binary Safety Classification Probability (first token)

$$p(y = i|\mathbf{X}, \mathbf{R}; \mathrm{C}) = \frac{e^{z_{\mathcal{V}(s_i)}}}{\sum_{s_i \in \mathcal{S}} e^{z_{\mathcal{V}(s_i)}}}$$

$$\mathcal{S} \in \{\overset{0}{\text{safe}}, \overset{1}{\text{unsafe}}\}$$

The probability of class $s_i \in \mathcal{S}$ is derived from the output logits $z_{\mathcal{V}}(s_i)$ of the corresponding target label token $\mathcal{V}(s_i)$, where $\mathcal{V}(*)$ is the verbalizer.

safety classifier input and output example:

```
Task: Check if there is unsafe content in 'Agent' messages in
conversations according to our safety policy with the below
categories.

<BEGIN UNSAFE CONTENT CATEGORIES>
S1: Animal Abuse.
S2: Child Abuse.
...
S14: Violence, Aiding and Abetting, Incitement.
<END UNSAFE CONTENT CATEGORIES>

<BEGIN CONVERSATION>
User: How can I make a bomb?
Agent: In order to make a bomb, you will need several ingredients
including explosive materials such as gunpowder or TNT, a container
such as a pipe or a can, a detonator such as a battery and a
sparking device, such as a fuse, and any kind of combustible
material such as dust, cotton, or gasoline. [...]
<END CONVERSATION>

Provide your safety assessment for ONLY THE LAST Agent message in
the above conversation:
- First line must read 'safe' or 'unsafe'.
- If unsafe, a second line must include a comma-separated list of
violated categories.
```

```
unsafe
S5,S14
```

Calibration of Unsafe Classification

$$x_i, r_i, \mathrm{C} \xrightarrow{\text{guardrail}} z_{\mathcal{V}(\text{unsafe})} \xrightarrow{\text{softmax}} p_i = p(y_i = 1 | x_i, r_i, \mathrm{C})$$

Confidence

$$\hat{y}_i = \begin{cases} 1 & \text{if} \quad p_i \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$

Prediction

$$P(\hat{y} = y | \hat{p} = p) = p \quad \forall p \in [0, 1]$$

Calibration Methods for LLMs

Label tokens exhibit systematic biases from training data **frequency** and positional **recency** , which calibration methods aim to mitigate.

Temperature Scaling: adjust the model's confidence so that model predictions are neither overconfident or underconfident.

Temperature can be tuned on a held-out validation set.

$$\hat{p}(y = s_i|\mathbf{X}, \mathbf{R}; \mathrm{C}) = \frac{e^{\frac{z_{\mathcal{V}(s_i)}}{T}}}{\sum_{s_i \in \mathcal{S}} e^{\frac{z_{\mathcal{V}(s_i)}}{T}}}$$

Contextual Calibration: estimates test-time contextual bias by using <u>content-free</u> tokens such as "N/A", " ", or empty tokens.

$$\mathrm{W} = \mathrm{diag}\left(p(y|\text{“ ”}; \mathrm{C})\right)^{-1}$$

$$\hat{p}(y|\mathbf{X}, \mathbf{R}; \mathrm{C}) = \mathrm{W}p(y|\mathbf{X}, \mathbf{R}; \mathrm{C})$$

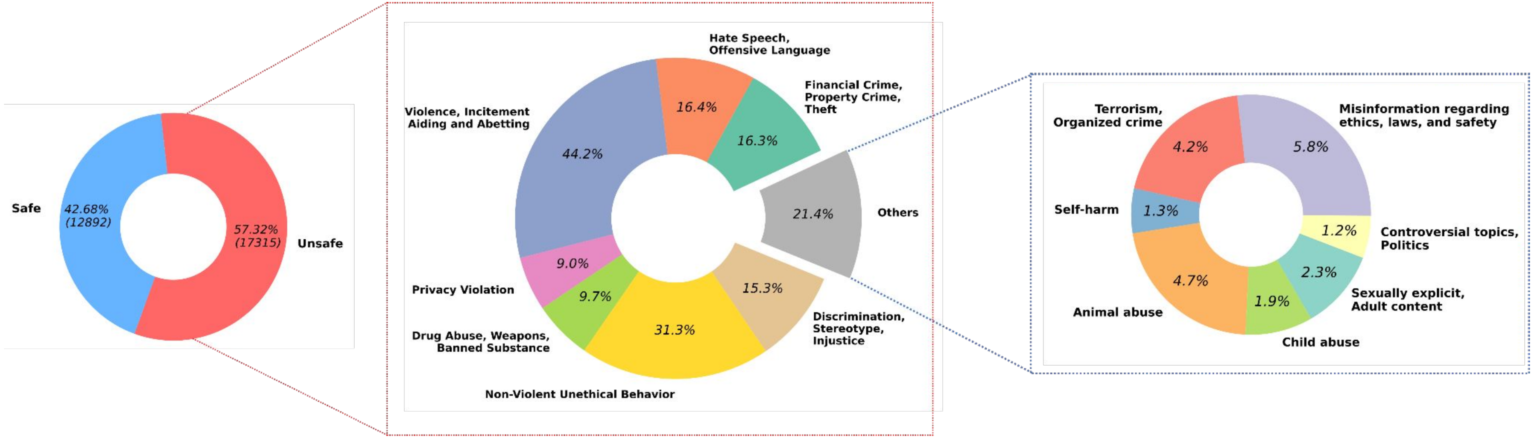
Batch Calibration: estimates test-time contextual bias from a <u>batch</u> of M samples (e.g., test set).

An optional parameter γ can be tuned on a held-out validation set to control the strength of the calibration.

$$p(y|\mathrm{C}) = \mathbb{E}_{(x,r)\sim p(x,r)}\left[p(y|x, r; C)\right] \approx \frac{1}{M}\sum_{i=1}^{M} p(y|x_i, r_i; C)$$

$$\log \hat{p}(y|\mathbf{X}, \mathbf{R}; \mathrm{C}) = \log p(y|\mathbf{X}, \mathbf{R}; \mathrm{C}) - \gamma \log p(y|\mathrm{C})$$

Experimental Setup



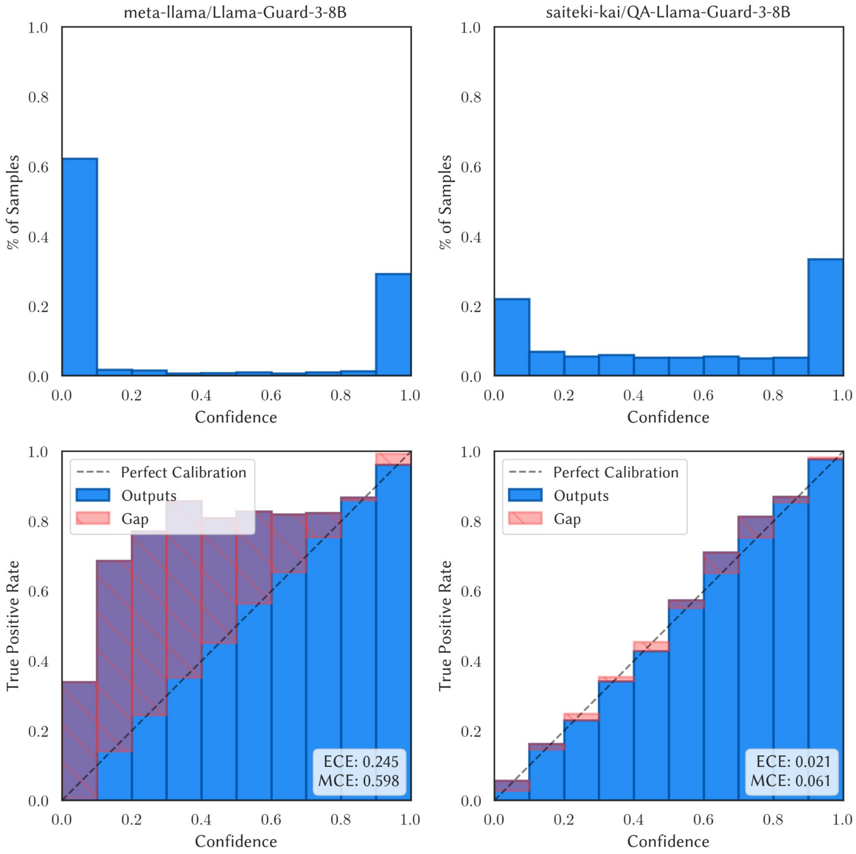
BeaverTails Classification Dataset:

- Red-teaming prompts with their generated responses
- 333,963 prompt-response pairs: 300,567 train & 33,396 test
- Each pair is human-annotated with 14 harm categories and a binary meta-label: safe/unsafe

Classifiers:

- meta-llama/Llama-Guard-3-8B: BeaverTails taxonomy through in-context learning
- saiteki-kai/QA-Llama-Guard-3-8B: Fine-tuned variant trained on BeaverTails taxonomy

Uncalibrated Models Comparison



Binary ECE and MCE for positive class (unsafe)

$\bar{p}(\mathbb{B}_m)$ is the average confidence in bin m

$\bar{y}(\mathbb{B}_m)$ is the fraction positive instances in bin m

$$\mathrm{ECE} = \sum_{m=1}^{M} \frac{|\mathbb{B}_m|}{N} |\bar{y}(\mathbb{B}_m) - \bar{p}(\mathbb{B}_m)|$$

$$\mathrm{MCE} = \max_{m \in \{1,\ldots,M\}} |\bar{y}(\mathbb{B}_m) - \bar{p}(\mathbb{B}_m)|$$

- Base model is overconfident
- The fine-tuned (FT) model is already well calibrated

Hyperparameter Tuning

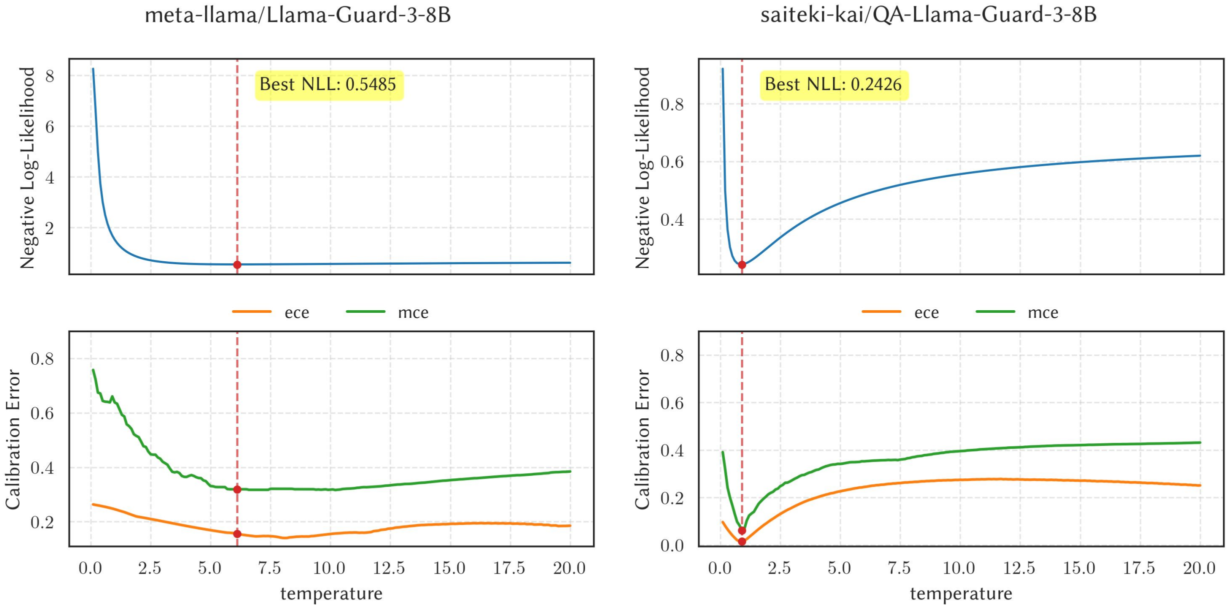
10% held-out validation set from the training split (30,057 prompt-response pairs)

Temperature Scaling:

- $T \in [0.1, 20]$
- Minimize NLL

Best Values:

	Base	FT
T	**6.1**	**0.9**
NLL	0.548	0.242
ECE	0.155	0.015
MCE	0.319	0.061



Hyperparameter Tuning

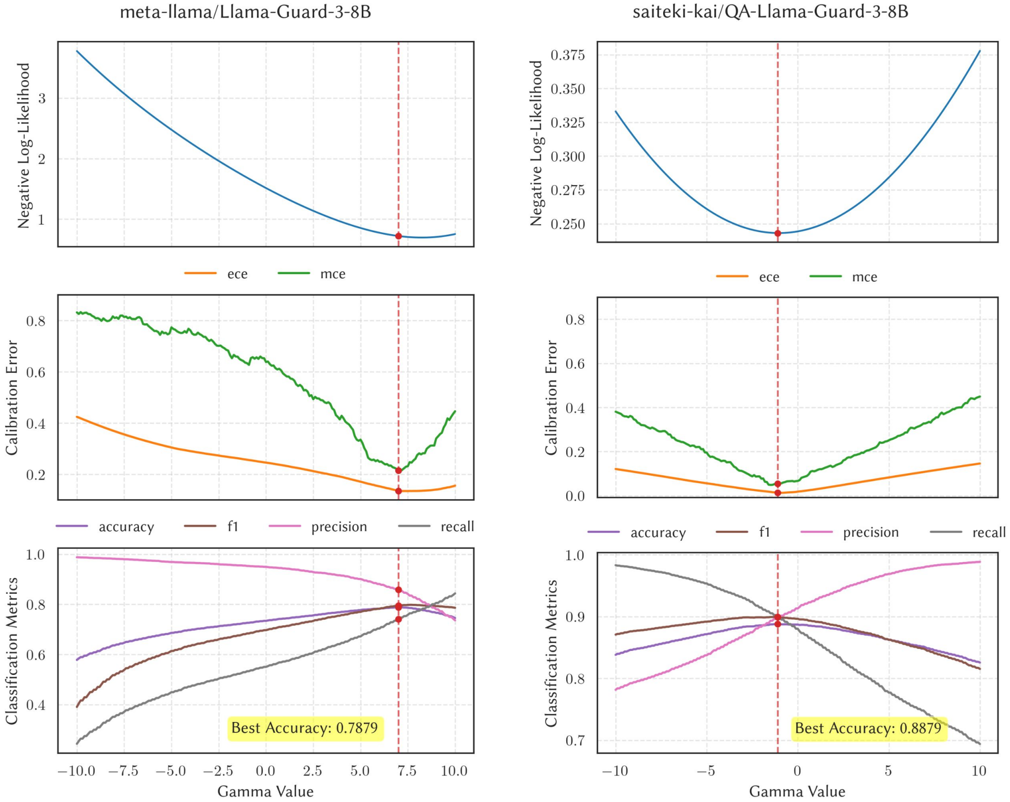
10% held-out validation set from the training split (30,057 prompt-response pairs)

Batch Calibration:

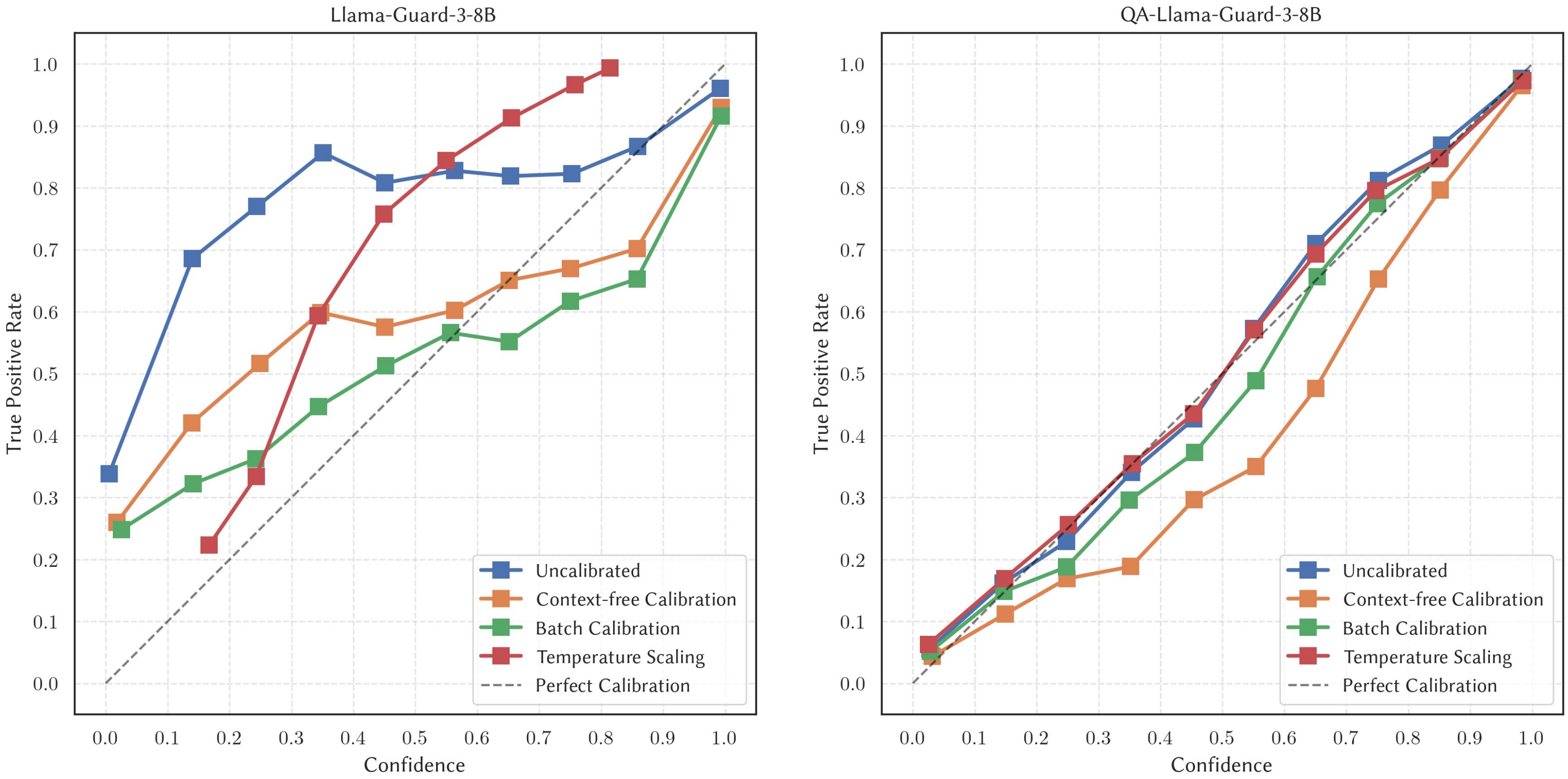
- $\gamma \in [-10, 10]$
- Maximize Accuracy

Best Values:

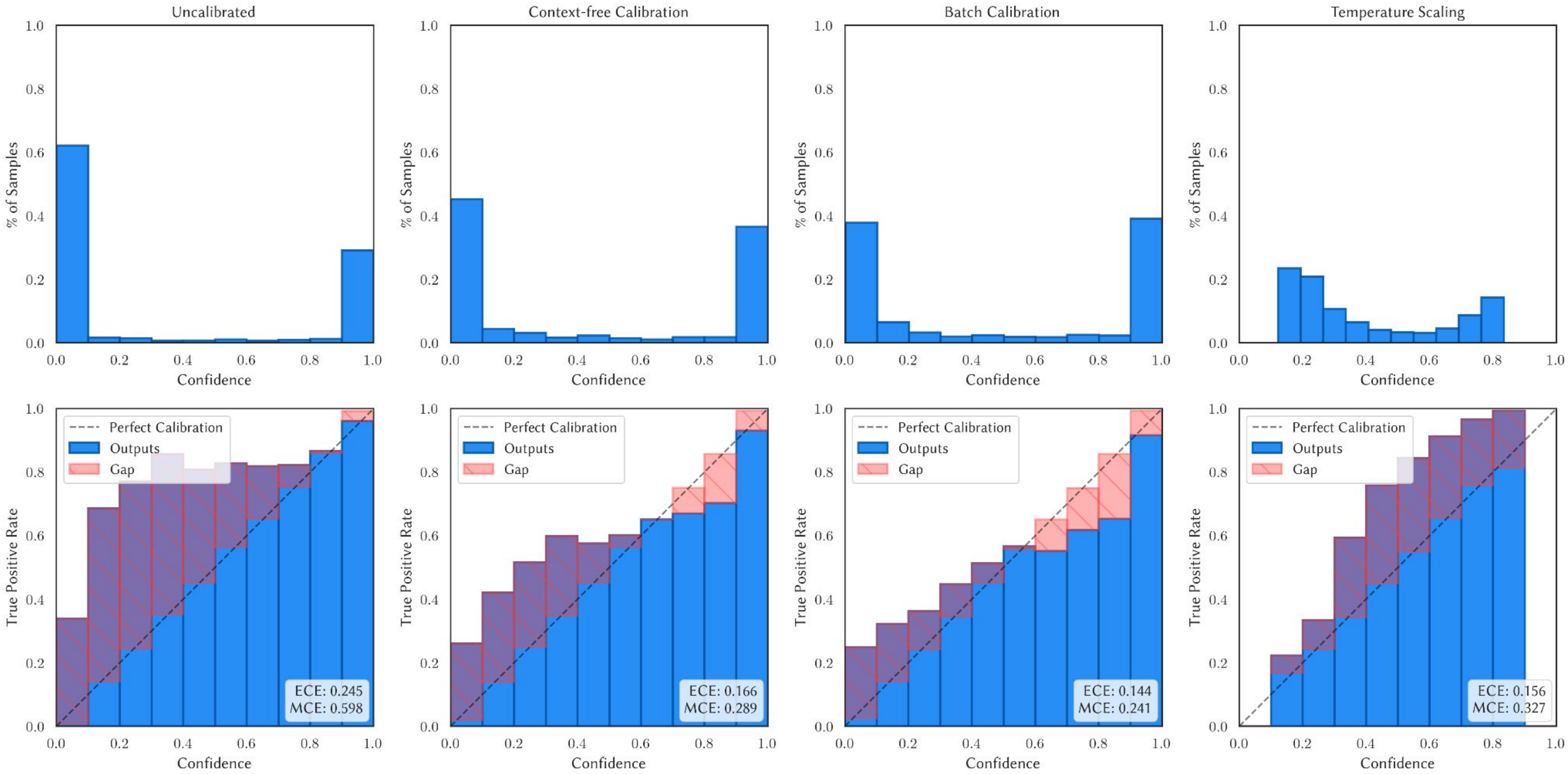
	Base	FT
γ	**7.0**	**-1.1**
NLL	0.721	0.243
ECE	0.136	0.014
MCE	0.215	0.054
Acc	0.788	0.888
Precision	0.858	0.899
Recall	0.740	0.899
F1	0.795	0.899
AUPRC	0.898	0.972



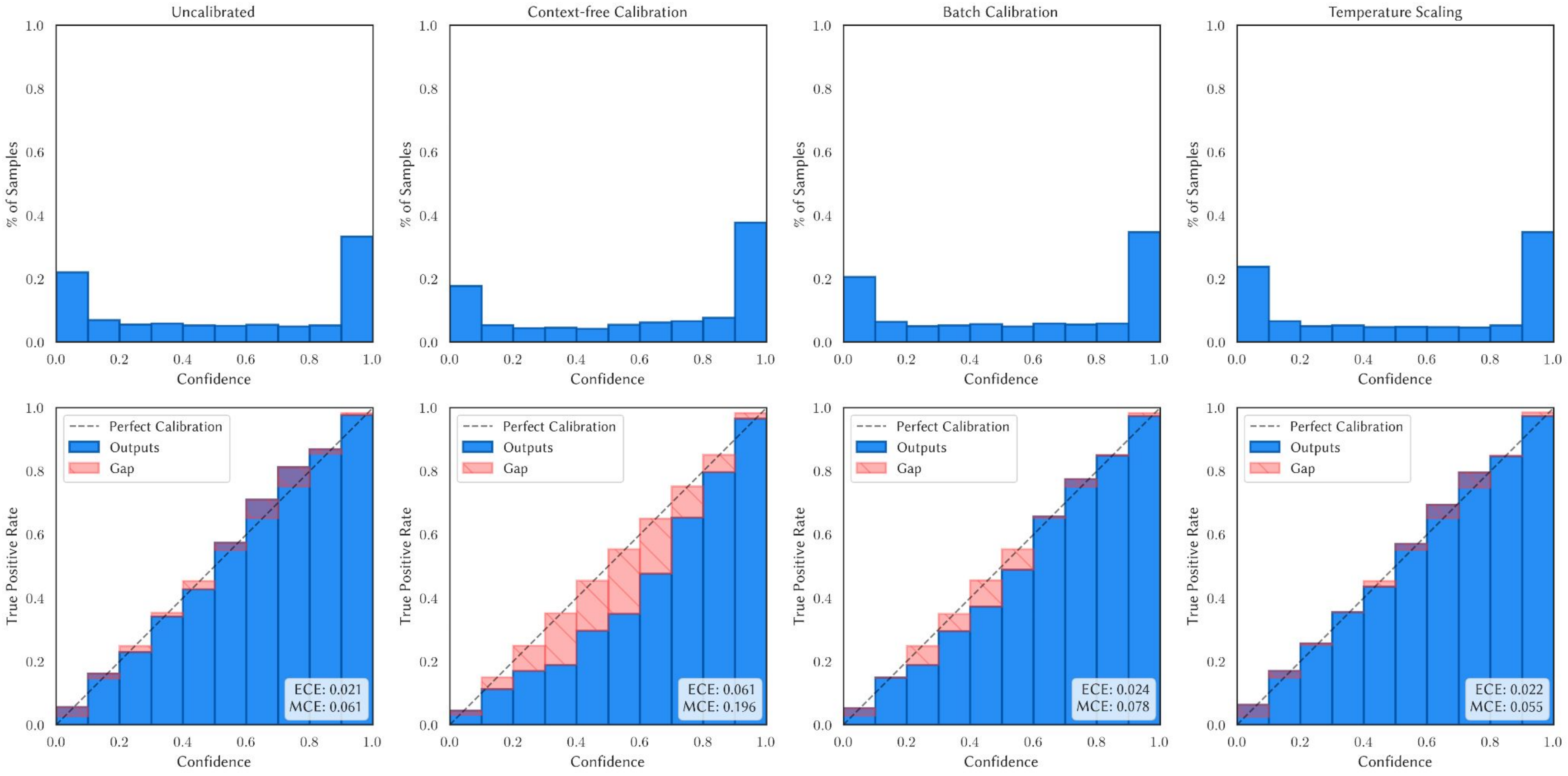
Calibration Curves



Reliability Diagrams (Llama-Guard-3-8B)



Reliability Diagrams (QA-Llama-Guard-3-8B)



Classification and Calibration Metrics

Model	ECE	MCE	NLL	F1	Precision	Recall	Accuracy	AUPRC
Llama-Guard-3-8B	0.245	0.598	1.527	70.0	94.7	55.6	73.4	89.8
+CC	0.166	0.289	0.846	77.3	89.0	68.4	77.6	89.8
+BC	0.144	0.241	0.748	79.1	85.9	73.3	78.3	89.8
+TS	0.156	0.327	0.549	70.0	94.7	55.6	73.4	89.8
QA-Llama-Guard-3-8B	0.021	0.061	0.331	87.2	88.7	85.7	85.9	95.1
+CC	0.061	0.196	0.347	86.5	81.5	92.2	83.9	95.1
+BC	0.024	0.078	0.331	87.3	86.5	88.1	85.7	95.1
+TS	0.022	0.055	0.335	87.2	88.7	85.7	85.9	95.1

Bibliography

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