Improving the Calibration of Confidence Scores in Text Generation Using the Output Distribution's Characteristics

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Abstract

Well-calibrated model confidence scores can improve the usefulness of text generation models. For example, users can be prompted to review predictions with low confidence scores, to prevent models from returning bad or potentially dangerous predictions. However, confidence metrics are not always well calibrated in text generation. One reason is that in generation, there can be many valid answers, which previous methods do not always account for. Hence, a confident model could distribute its output probability among multiple sequences because they are all valid. We propose taskagnostic confidence metrics suited to generation, which rely solely on the probabilities associated with the model outputs without the need for further fine-tuning or heuristics. Using these, we are able to improve the calibration of BART and Flan-T5 on summarization, translation, and QA datasets.

1 Introduction

Confidence scores are scores derived from a model's output, which are interpreted as the model's estimation of its own output's quality. These scores can be used in real-world applications to flag uncertain predictions in automated decision-making systems (Malinin and Gales, 2021), which could prompt further human review (Xiao et al., 2020), or force the model to abstain from answering when unsure (Liu et al., 2020; Kamath et al., 2020). To be useful, we want these scores to correlate with the output's quality.

A common approach to estimating confidence is through probability-based methods, which rely on the probabilities assigned by the model to output tokens. Most existing methods focus on the sequence with the highest probability, which we refer to as the top sequence (Murray and Chiang, 2018; Zablotskaia et al., 2023; Huang et al., 2023; Zhao et al., 2020; Perlitz et al., 2023; Malinin and Gales,

2021). A high probability for the top sequence suggests strong confidence in a particular prediction, while a lower value indicates uncertainty.

This approach is effective for tasks with a single correct answer. However, it faces significant challenges when applied to tasks with multiple valid outputs, as in many generation tasks. In such cases, a low top probability may not reflect a lack of confidence but rather that the model has identified several valid sequences (See Figure 1). Ideally, for open-ended tasks, a confident model would distribute high probabilities across multiple good sequences while assigning lower probabilities to less suitable options, while in classification, confidence can be indicated by a single high top probability.

To address this limitation, we propose new probability-based confidence estimation methods that consider the probabilities of multiple sequences instead of focusing solely on the top one. We introduce two methods: the first calculates the probability ratio between the highest-ranked sequences and the rest, while the second evaluates the thinness of the distribution's tail. Our experiments demonstrate that these metrics outperform existing baselines across three open-ended text generation tasks: translation, QA, and summarization.

2 Related Work

Probability-Based Methods These methods rely on the model outputs to compute token-level probabilities or entropy (Murray and Chiang, 2018; Zablotskaia et al., 2023; Zhao et al., 2020; Perlitz et al., 2023; Kumar and Sarawagi, 2019; Huang et al., 2023; Malinin and Gales, 2021). Other work uses natural language inference models to group similar sequences before computing entropy (Lin et al., 2023; Kuhn et al., 2023; Nikitin et al., 2024).

Similarity/Disagreement Based Methods When answers can be sampled from models (e.g., through dropout), self-consistency can be used

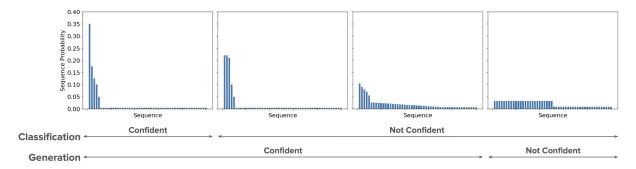


Figure 1: We illustrate the difference in interpretation of confidence in classification vs generation. Suppose a model generated output probability distributions for four different inputs; each bar is the prob. assigned to one class/sequence. In classification, only the 1st output would show model confidence, as it assigned most probability to one class. In generation, the first 3 outputs *could* show confidence because multiple sequences were valid.

to measure confidence: consistency across the top answers indicates confidence while variance indicates uncertainty (Xiao et al., 2020; Schmidt et al., 2022; Lakshminarayanan et al., 2017).

Fine-Tuning Based Methods In addition, other methods also fine-tune additional models to predict the correctness or confidence of the output (Yaldiz et al., 2024; Kamath et al., 2020; Malinin et al., 2019; Fathullah et al., 2023).

Out of Distribution Detection (OOD) Methods

OOD can also be used to detect if a sample is in the training distribution, in which case a model is assumed to be confident (Liu et al., 2020; Vazhentsev et al., 2023).

Verbalized Confidence Scores With the increased conversational ability of LLMs, recent work prompts the model to give a confidence score with its answer (Lin et al., 2022; Tian et al., 2023; Kapoor et al., 2024; Han et al., 2024).

Our work is closest to the probability-based methods; they are easily adaptable and task agnostic. They do not require metrics or NLI models to measure similarity, computation for OOD detection, or models that can verbalize their confidence.

3 Method

Problem Definition We define confidence as a score computed using the model outputs, that describes its assessment of its prediction quality. We want to compute the model's sample-level confidence for its output, that is positively correlated (i.e. calibrated) to the output's quality, measured by the evaluation metric used for the task (e.g. automated

metrics, human evaluation). Formally,

Confidence
$$(x, \hat{y}, \phi) \propto \text{Quality}(y, \hat{y}),$$

where x is the input, y is the target, \hat{y} is the prediction, and ϕ are the model parameters.

At inference time, we run beam search to generate N sequences. Each sequence's probability is obtained by taking the product of the individual token probabilities. Given the i-th beam $\hat{y}^{(i)}$:

$$p_{\hat{y}^{(i)}}(x) = \prod_{t} p(\hat{y}_{t}^{(i)} | \hat{y}_{< t}^{(i)}, x)$$

Methods We account for the fact that there can be multiple valid outputs by measuring two characteristics that we hypothesize are present in all confident outputs regardless of the number of valid sequences (See Figure 2). The first characteristic of a confident model is that it distinguishes good from average or bad sequences, and subsequently assigns higher probability to a select set of sequences it deems as good compared to other sequences.

Ratio This motivates the ratio method: we measure how much more confident the model is in one of its *best* beams $p_{\hat{y}^{(1)}}$, versus one of its *average* beams $p_{\hat{y}^{(k)}}$, where $p_{\hat{y}^{(1)}}$ to $p_{\hat{y}^{(k)}}$ are sorted in descending order. This captures the intuition that a confident model will assign more probability to its best sequence than to an average sequence, whereas an unconfident model would assign similar probabilities to them. We expect the optimal value of k to differ by task, as different tasks can have different levels of diversity in valid generation outputs. Hence, we tune k on a validation set, and report its performance on the test set in the results.

$$\operatorname{Ratio}(x) = \frac{p_{\hat{y}^{(1)}}(x)}{p_{\hat{y}^{(k)}}(x)}$$

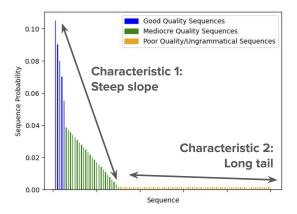


Figure 2: We hypothesize that a confident model's output *would* have a steep slope and long tail; colors added for illustration purposes only.

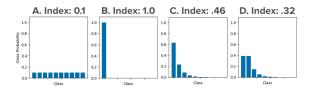


Figure 3: Samples of distributions and their tail indices

The second characteristic of a confident model is that it will assign low probability to many *bad* sequences. Suppose each sequence is a "class" – in Figure 3B, 3C, and 3D, the right-most classes have very small probabilities, and hence have a "thin tail"; all three figures exhibit this property, regardless of how many *correct* sequences they have. In contrast, an unconfident output where all classes receive equal probability (Figure 3A) has a thick tail. We quantify this with the tail index.

Tail Thinness We adapt the tail index proposed by Huang (2024), originally designed to measure the thinness of statistical distributions. The higher the tail thinness, the thinner the tail.

Tail Thinness
$$(x) = \sum_{i=1}^{N} p_{\hat{y}^{(i)}}(x)^2$$

This sums the squared sequence probabilities for all N sequences generated using beam search. Because the probabilities for N sequences do not sum to 1, we first normalize them using softmax. We report the temperature used in Appendix A. Applying this to Figure 3, the uniform distribution (Fig A) gets a small tail thinness, while a degenerate distribution (Fig B) has the highest tail thinness. The metric also assigns similar scores to distributions with similar tail thicknesses (Figs C and D). While

this performs similarly to sequence-level entropy (Appendix C), we use tail-thinness metric (Huang, 2024) as it better describes the shape of the tail for which we have formulated our assumptions.

4 Experiments

Fine-tuning and Inference We first perform supervised fine-tuning (SFT) with BART Base (Lewis et al., 2019) or Flan-T5 Base (Chung et al., 2022), both relatively small models with no prior ability to verbalize confidence (Appendix A). After SFT, we generate the confidence scores for the test set. We get the sequence probabilities the top N=100 sequences, using beam search from HuggingFace (Wolf et al., 2020), and replicate the baselines.

Evaluation We compute the Spearman correlation between the confidence scores and the quality scores, similar to analyses by Zablotskaia et al. (2023); Malinin and Gales (2021). We evaluate the top beam against the reference using ROUGE-L (Lin, 2004) for summarization, BLEU (Papineni et al., 2002) for translation, or F1 for question answering, and test for statistical significance with a bootstrap test (Berg-Kirkpatrick et al., 2012).

Baselines We report the equations that we replicate from previous literature, shown in Table 1.

For the probability based methods (Rows 1-4), we compute (1) ATP: average token probability for the top sequence (Murray and Chiang, 2018; Zablotskaia et al., 2023), (2) ATE: average token entropy for the top sequence (Zhao et al., 2020; Perlitz et al., 2023), (3) DAE: dropout-based average token entropy across 10 outputs (Eq 1) (Malinin and Gales, 2021), and (4) WTP: weighted average of the top-K sequences' average token log probabilities (Eq 2) (Malinin and Gales, 2021).

For the similarity/disagreement based methods (Rows 5-7), we use dropout and sample 10 outputs per instance. We compute the (1) DSM: dropout similarity using METEOR (Eq 3) (Schmidt et al., 2022), (2) DVB: dropout variance using BLEU (Eq 4) (Xiao et al., 2020), and (3) DVK: dropout variance between token probabilities using KL divergence (Eq 5) (Lakshminarayanan et al., 2017).

$$\mathrm{Conf}_{\mathrm{DAE}} = \frac{1}{10} \sum_{i=1}^{10} \frac{1}{|\hat{y}^{(i)}|} \sum_{t=1}^{|\hat{y}^{(i)}|} \mathcal{H}\left(p(\hat{y}_t^{(i)}|\hat{y}_{< t}^{(i)}, x)\right) \tag{1}$$

$$\begin{split} \mathcal{H}\left(p(\hat{y}_t^{(i)}|\hat{y}_{< t}^{(i)}, x)\right) = \\ &- \sum_{i=1}^{|\mathcal{V}|} p(\hat{y}_{t, j}^{(i)}|\hat{y}_{< t}^{(i)}, x) \text{log}\left(p(\hat{y}_{t, j}^{(i)}|\hat{y}_{< t}^{(i)}, x)\right) \end{split}$$

$$\begin{aligned} & \operatorname{Conf}_{\operatorname{WTP}} = -\sum_{i=1}^{10} \pi_i \left(\frac{1}{|\hat{y}^{(i)}|} \ln(p(\hat{y}^{(i)})) \right) & \qquad (2) \\ & \pi_i = \frac{\exp\left(\frac{1}{|\hat{y}^{(i)}|} \ln(p(\hat{y}^{(i)})) \right)}{\sum_{j=1}^{10} \exp\left(\frac{1}{|\hat{y}^{(j)}|} \ln(p(\hat{y}^{(i)})) \right)} \\ & \ln(p(\hat{y}^{(i)})) = \sum_{t=1}^{|\hat{y}^{(i)}|} \ln(p(\hat{y}^{(i)}_t|\hat{y}^{(i)}_{< t}, x)) \\ & \operatorname{Conf}_{\operatorname{DSM}} = \frac{\sum_{i=1}^{10} \sum_{j=1}^{10} \operatorname{Meteor}(\hat{y}^{(i)}, \hat{y}^{(j)})}{N(N-1)} & \qquad (3) \\ & \operatorname{Conf}_{\operatorname{DVB}} = \sum_{i=1}^{10} \sum_{j=1}^{10} (1 - \operatorname{BLEU}(\hat{y}^{(i)}, \hat{y}^{(j)}))^2 & \qquad (4) \end{aligned}$$

$$\operatorname{Conf}_{\text{DVK}} = \sum_{i=1}^{10} KL(p(\hat{y}^{(i)}|x), p_{\hat{y}}) \qquad (5)$$

$$\bar{y}_{\text{Prob}} = \frac{1}{10} \sum_{i=1}^{10} p(\hat{y}^{(i)}|x)$$

Where $\hat{y}^{(i)}$ is the decoded sequence i sampled by activating dropout, $\hat{y}_t^{(i)}$ is the t-th output token for sequence i, and $\hat{y}_{t,j}^{(i)}$ is the j-th vocabulary at position t for sequence i.

Datasets We test on **Translation** (1) WMT 2017 English-German (Bojar et al., 2017), (2) WMT 2017 English-Russian (Bojar et al., 2017), (3) FLO-RES (Filipino Set) (NLLB, 2022), **Question Answering** (1) SQUAD (Rajpurkar et al., 2016), (2) HotpotQA (Yang et al., 2018), **Summarization** (1) DebateSumm (Roush and Balaji, 2020), (2) Reddit-TiFu (Kim et al., 2018), (3) XSUM (Narayan et al., 2018), (4) CNN-DailyMail (See et al., 2017)

5 Results

We report the correlation between the evaluation metric and confidence scores in Table 1 (See Appendix A for details). For BART, our methods achieve better correlation on 6 out of 9 datasets. We see larger gains in translation and question answering, as compared to summarization. The tail thinness method generally yields larger improvements (up to +17.2%) than the ratio method (up to +16.1%). For Flan-T5, our methods also achieve better correlation on 4 out of 9 datasets. Like for BART, we observe larger improvements using the tail thinness (up to +10.0%) method than the ratio based method (up to +8.3%). Overall, our methods yield the best performance more frequently than previous methods across all dataset-model pairs (tail thinness: 10/16, ratio: 8/16, DSM: 4/16), with median rankings of 2 and 3 for the tail and ratio methods (next being ATP, rank 4).

Robustness to Multiple Valid Sequences tatively, we find that our methods assign high confidence to outputs where there are multiple valid sequences. We look at examples where our metrics assigned high confidence, but other methods like average token log probability assigned low confidence (See Figure 4). In these examples, there were indeed multiple, correct outputs; this resulted in lower probability for the top beam (2nd and 3rd image). If we only used the top beam's probability to measure confidence, we might conclude that the model is unconfident. In contrast, our methods which rely on the ratio of sequence probabilities and tail thinness, rather than the top probability, are able to correctly identify that the model is still confident in such scenarios. This illustrates how using features of the distribution like slope or tail thinness can be more indicative of confidence in text generation, rather than solely looking at the features of the top output.

Failure Cases We examine samples for which the confidence scores are not well calibrated. Looking at the FLORES (Filipino) for Flan-T5, we observed samples where the model was confident, but its output was bad. Here, the model failed to translate a few key terms, which changed the meaning of the sentence (See Table 6). Other times, the confidence scores were well calibrated, but the quality score was not estimated well. This stemmed from noisy labels or limitations of the evaluation metric (See Table 7) which may require future work.

Choice of k In general, open ended tasks (translation, summarization) benefited from larger values for k, and close-ended tasks (QA) from smaller values of k (See Figure 5). One explanation for this could be that k serves as a parameter which delineates the good vs. average sequences. Finding the k that best separates the two groups allows us to most accurately measure the difference in confidence between both groups. Open-ended tasks can have more good sequences, hence correlation is maximized when we choose a higher value for k. In contrast, close-ended tasks have fewer good sequences, so a lower value for k is better.

We note that the optimal value for k may be very large for open-ended tasks like summarization. In our experiments, we capped k to 100 due to computational limitations, which may have underestimated its optimal value, and thus explain why our methods are less competitive than the baselines.

		Fil-	EN	DE-	EN	RU-	EN	Hotp	ootQA	SQU	AD	De	bate	Red	ddit (CNN		XSUM		ınk
		Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Avg	Med
- T	ATP	.473	.468	.028	.370	.530	.023	.209	.302	.391	.577	.447	.247	.618	.577	.109	.156	.119	.078	4.4	4
Þi	ATE	.308	.335	.035	.297	.437	.042	.051	.152	.094	.049	.416	.248	.615	.474	.020	.138	.093	.082	6.4	7
oba	DAE	.217	.161	.346	.294	.230	.178	.242	.367	.327	.226	.135	.037	.049	.049	.295	.380	.314	.353	5.4	6
Pro	WTP	.516	.495	.162	.287	.602	.055	.130	.180	.179	.020	.489	.253	.616	.575	.106	.162	.120	.063	5	5
Ħ	DSM	.441	.508	.424	.462	.374	.486	.168	.270	.394	.332	.192	.038	.038	.167	.255	.323	.323	.383	4.4	4.5
Ş	DVB	.455	.489	.512	.461	.409	.488	.043	.000	.378	.467	.144	.061	.058	.143	.264	.325	.305	.363	4.7	4.5
Sin	DVK	.001	.008	.110	.064	.110	.013	.177	.232	.340	.426	.063	.025	.045	.059	.065	.070	.103	.117	7.6	8
LIS	Ratio	.546	.200	*.653	.209	*.768	.491	.249	.360	*.505	.565	.496	☆.293	.596	.304	.103	.055	.082	.196	3.9	3
Õ	Tail	*.649	.380	*.648	.190	*. 779	.506	.255	*.451	*.493	.582	.518	*.354	.601	.300	.100	.031	.131	.212	3.2	2

Table 1: Spearman correlation (absolute value) between confidence score and evaluation metric/quality score (BLEU for translation, F1 for QA, RougeL for summarization); Bt: BART, FT5: Flan-T5, stars indicate significant difference from next best method (bootstrap test, $\alpha = 0.10$, $\alpha = 0.05$)

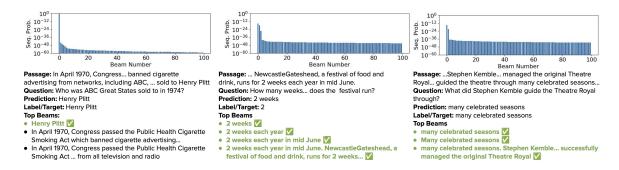


Figure 4: Samples from SQUAD (Rajpurkar et al., 2016); 1st image only has one valid output, whereas the 2nd and 3rd have multiple; our tail-thinness and ratio based confidence correctly assign high confidence to all samples, but avg. log prob. only assigns high confidence to the first image (Note: The y-axis is plotted on the log scale)

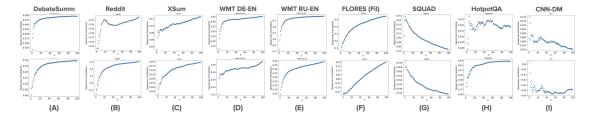


Figure 5: Spearman Correlation vs k on test set for BART (top row) and Flan-T5 (bottom row); In general, openended tasks (summarization: A-C, translation: D-F) benefit from larger k, close-ended tasks (QA: G-H, Reddit: I) use smaller k

6 Conclusion

We identified characteristics of output distributions from a confident model in generation tasks, and used this to propose metrics that capture these characteristics. We find that on various datasets, these characteristics are better correlated to quality metrics than previous methods.

There are various directions future work can take to improve the computation and evaluation of confidence scores. For example, we observed that models can be overly confident in wrong answers (Table 6), which can lead to miscalibration when using our methods. Future work can study the reasons for model overconfidence, and propose ways

to reduce or account for this. In addition, more work is required to improve the evaluation of calibration in generation tasks. Concretely, calibration is well defined for classification tasks when there is a binary outcome, and metrics like expected calibration error (Tian et al., 2023) measure whether the model's confidence scores match its accuracy (e.g. A model should be right in 90% of the examples for which it claimed to be 90% confident). More work can be done to develop metrics that capture a similar notion of calibration in generation tasks where the outcome is continuous.

Limitations and Potential Risks

One limitation is that our methods require users to compute k beams, both when tuning hyperparameters, and at inference time. This can be computationally expensive, especially for open-ended tasks where the optimal value of k may be large. Hence, future work may find more efficient ways of estimating the confidence.

Another caveat is that we only evaluate the performance of our methods on a limited set of models and parameters. For example, we fine-tuned various models with early stopping. Hence, future work which seeks to use these methods must reevaluate the scores on their tasks, to avoid deploying miscalibrated confidence scores in practical settings.

Finally, future work could study better ways to evaluate confidence scores; we found that traditional evaluation metrics may lead to poor quality ratings, and it was difficult to find datasets with human evaluation scores to use.

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References

Taylor Berg-Kirkpatrick, David Burkett, and Dan Klein. 2012. An empirical investigation of statistical significance in NLP. In *Proceedings of the 2012 Joint Conference on Empirical Methods in Natural Language Processing and Computational Natural Language Learning*, pages 995–1005, Jeju Island, Korea. Association for Computational Linguistics.

Ond rej Bojar, Rajen Chatterjee, Christian Federmann, Yvette Graham, Barry Haddow, Shujian Huang, Matthias Huck, Philipp Koehn, Qun Liu, Varvara Logacheva, Christof Monz, Matteo Negri, Matt Post, Raphael Rubino, Lucia Specia, and Marco Turchi. 2017. Findings of the 2017 conference on machine translation (wmt17). In *Proceedings of the Second Conference on Machine Translation, Volume 2: Shared Task Papers*, pages 169–214, Copenhagen, Denmark. Association for Computational Linguistics.

Hyung Won Chung, Le Hou, Shayne Longpre, Barret Zoph, Yi Tay, William Fedus, Eric Li, Xuezhi Wang, Mostafa Dehghani, Siddhartha Brahma, Albert Webson, Shixiang Shane Gu, Zhuyun Dai, Mirac Suzgun, Xinyun Chen, Aakanksha Chowdhery, Sharan Narang, Gaurav Mishra, Adams Yu, Vincent Zhao, Yanping Huang, Andrew Dai, Hongkun Yu, Slav Petrov, Ed H. Chi, Jeff Dean, Jacob Devlin, Adam Roberts, Denny Zhou, Quoc V. Le, and Jason Wei. 2022. Scaling instruction-finetuned language models.

Yassir Fathullah, Guoxuan Xia, and Mark John Francis Gales. 2023. Logit-based ensemble distribution distillation for robust autoregressive sequence uncertainties. *ArXiv*, abs/2305.10384.

Haixia Han, Tingyun Li, Shisong Chen, Jie Shi, Chengyu Du, Yanghua Xiao, Jiaqing Liang, and Xin Lin. 2024. Enhancing confidence expression in large language models through learning from past experience.

Hening Huang. 2024. A new measure of the tail-heaviness of a probability distribution.

Yuheng Huang, Jiayang Song, Zhijie Wang, Shengming Zhao, Huaming Chen, Felix Juefei-Xu, and Lei Ma. 2023. Look before you leap: An exploratory study of uncertainty measurement for large language models.

Amita Kamath, Robin Jia, and Percy Liang. 2020. Selective question answering under domain shift. In *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*, pages 5684–5696, Online. Association for Computational Linguistics.

Sanyam Kapoor, Nate Gruver, Manley Roberts, Katherine Collins, Arka Pal, Umang Bhatt, Adrian Weller, Samuel Dooley, Micah Goldblum, and Andrew Gordon Wilson. 2024. Large language models must be taught to know what they don't know.

Byeongchang Kim, Hyunwoo Kim, and Gunhee Kim. 2018. Abstractive summarization of reddit posts with multi-level memory networks.

Lorenz Kuhn, Yarin Gal, and Sebastian Farquhar. 2023. Semantic uncertainty: Linguistic invariances for uncertainty estimation in natural language generation. In *The Eleventh International Conference on Learning Representations*.

Aviral Kumar and Sunita Sarawagi. 2019. Calibration of encoder decoder models for neural machine translation. *ArXiv*, abs/1903.00802.

Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. 2017. Simple and scalable predictive uncertainty estimation using deep ensembles.

Mike Lewis, Yinhan Liu, Naman Goyal, Marjan Ghazvininejad, Abdelrahman Mohamed, Omer Levy, Veselin Stoyanov, and Luke Zettlemoyer. 2019. BART: denoising sequence-to-sequence pre-training

- for natural language generation, translation, and comprehension. *CoRR*, abs/1910.13461.
- Chin-Yew Lin. 2004. ROUGE: A package for automatic evaluation of summaries. In *Text Summarization Branches Out*, pages 74–81, Barcelona, Spain. Association for Computational Linguistics.
- Stephanie Lin, Jacob Hilton, and Owain Evans. 2022. Teaching models to express their uncertainty in words. *Transactions on Machine Learning Research*.
- Zhen Lin, Shubhendu Trivedi, and Jimeng Sun. 2023. Generating with confidence: Uncertainty quantification for black-box large language models. *Trans. Mach. Learn. Res.*, 2024.
- Jeremiah Zhe Liu, Zi Lin, Shreyas Padhy, Dustin Tran, Tania Bedrax-Weiss, and Balaji Lakshminarayanan. 2020. Simple and principled uncertainty estimation with deterministic deep learning via distance awareness.
- Andrey Malinin and Mark Gales. 2021. Uncertainty estimation in autoregressive structured prediction.
- Andrey Malinin, Bruno Mlodozeniec, and Mark John Francis Gales. 2019. Ensemble distribution distillation. *ArXiv*, abs/1905.00076.
- Kenton Murray and David Chiang. 2018. Correcting length bias in neural machine translation. In *Proceedings of the Third Conference on Machine Translation: Research Papers*, pages 212–223, Brussels, Belgium. Association for Computational Linguistics.
- Shashi Narayan, Shay B. Cohen, and Mirella Lapata. 2018. Don't give me the details, just the summary! topic-aware convolutional neural networks for extreme summarization. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing*, pages 1797–1807, Brussels, Belgium. Association for Computational Linguistics.
- Alexander Nikitin, Jannik Kossen, Yarin Gal, and Pekka Marttinen. 2024. Kernel language entropy: Finegrained uncertainty quantification for llms from semantic similarities. *ArXiv*, abs/2405.20003.
- Team NLLB. 2022. No language left behind: Scaling human-centered machine translation.
- Kishore Papineni, Salim Roukos, Todd Ward, and Wei-Jing Zhu. 2002. Bleu: a method for automatic evaluation of machine translation. In *Proceedings of the* 40th Annual Meeting of the Association for Computational Linguistics, pages 311–318, Philadelphia, Pennsylvania, USA. Association for Computational Linguistics.
- Yotam Perlitz, Ariel Gera, Michal Shmueli-Scheuer, Dafna Sheinwald, Noam Slonim, and Liat Ein-Dor. 2023. Active learning for natural language generation. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 9862–9877, Singapore. Association for Computational Linguistics.

- Pranav Rajpurkar, Jian Zhang, Konstantin Lopyrev, and Percy Liang. 2016. SQuAD: 100,000+ questions for machine comprehension of text. In *Proceedings of the 2016 Conference on Empirical Methods in Natural Language Processing*, pages 2383–2392, Austin, Texas. Association for Computational Linguistics.
- Allen Roush and Arvind Balaji. 2020. DebateSum: A large-scale argument mining and summarization dataset. In *Proceedings of the 7th Workshop on Argument Mining*, pages 1–7, Online. Association for Computational Linguistics.
- Maximilian Schmidt, A. Bartezzaghi, Jasmina Bogojeska, Adelmo Cristiano Innocenza Malossi, and Thang Vu. 2022. Combining data generation and active learning for low-resource question answering. In *International Conference on Artificial Neural Net*works.
- Abigail See, Peter J. Liu, and Christopher D. Manning. 2017. Get to the point: Summarization with pointergenerator networks. In *Proceedings of the 55th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 1073–1083, Vancouver, Canada. Association for Computational Linguistics.
- Katherine Tian, Eric Mitchell, Allan Zhou, Archit Sharma, Rafael Rafailov, Huaxiu Yao, Chelsea Finn, and Christopher Manning. 2023. Just ask for calibration: Strategies for eliciting calibrated confidence scores from language models fine-tuned with human feedback. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 5433–5442, Singapore. Association for Computational Linguistics.
- Artem Vazhentsev, Akim Tsvigun, Roman Vashurin, Sergey Petrakov, Daniil Vasilev, Maxim Panov, Alexander Panchenko, and Artem Shelmanov. 2023. Efficient out-of-domain detection for sequence to sequence models. In *Findings of the Association for Computational Linguistics: ACL 2023*, pages 1430–1454, Toronto, Canada. Association for Computational Linguistics.
- Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, Joe Davison, Sam Shleifer, Patrick von Platen, Clara Ma, Yacine Jernite, Julien Plu, Canwen Xu, Teven Le Scao, Sylvain Gugger, Mariama Drame, Quentin Lhoest, and Alexander M. Rush. 2020. Huggingface's transformers: State-of-the-art natural language processing.
- Tim Z. Xiao, Aidan N. Gomez, and Yarin Gal. 2020. Wat zei je? detecting out-of-distribution translations with variational transformers.
- Duygu Nur Yaldiz, Yavuz Faruk Bakman, Baturalp Buyukates, Chenyang Tao, Anil Ramakrishna, Dimitrios Dimitriadis, and Amir Salman Avestimehr. 2024. Do not design, learn: A trainable scoring

function for uncertainty estimation in generative llms. *ArXiv*, abs/2406.11278.

Zhilin Yang, Peng Qi, Saizheng Zhang, Yoshua Bengio, William Cohen, Ruslan Salakhutdinov, and Christopher D. Manning. 2018. HotpotQA: A dataset for diverse, explainable multi-hop question answering. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing*, pages 2369–2380, Brussels, Belgium. Association for Computational Linguistics.

Polina Zablotskaia, Du Phan, Joshua Maynez, Shashi Narayan, Jie Ren, and Jeremiah Liu. 2023. On uncertainty calibration and selective generation in probabilistic neural summarization: A benchmark study. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 2980–2992, Singapore. Association for Computational Linguistics.

Yuekai Zhao, Haoran Zhang, Shuchang Zhou, and Zhihua Zhang. 2020. Active learning approaches to enhancing neural machine translation. In *Findings of the Association for Computational Linguistics: EMNLP 2020*, pages 1796–1806, Online. Association for Computational Linguistics.

A Implementation Details

All models were fine-tuned on one NVIDIA A100 GPU, with a constant learning rate 5e-5, and batch size of 10. The scripts and fine-tuned models are provided in the repository. Roughly 80 hours were used to train and perform inference on one GPU.

During SFT, we train for at most 3 epochs. We observe overfitting on many datasets, and remedy this by employing early stopping, where we stop training if the loss on the validation set does not improve after 2 steps. This was applied to all datasets except HotpotQA, WMT RU-EN, and DebateSumm. We report the number of SFT steps in Table 2.

Dataset	BART	Flan-T5
WMT DE-EN	200	200
WMT RU-EN	6000	6000
FLORES Filipino	260	200
SQUAD	220	240
HotpotQA	26835	26835
DebateSumm	1500	1500
Reddit	140	200
CNN	200	200
XSUM	120	200

Table 2: Number of Fine-Tuning Steps Taken per Task and Model

We report the parameters used for the ratio and tail-thinness methods (k: ratio method, temperature: softmax for the tail method) in Table 3.

Dataset	Model	k	Temp
FLORES Filipino	BART	99	1.000
	Flan-T5	99	1.000
WMT DE-EN	BART	99	1.000
	Flan-T5	99	1.000
WMT RU-EN	BART	79	1.000
	Flan-T5	99	1.000
HotpotQA	BART	1	0.010
	Flan-T5	1	0.050
SQUAD	BART	1	0.050
	Flan-T5	4	0.001
DebateSumm	BART	95	1.000
	Flan-T5	85	1.000
Reddit	BART	2	0.005
	Flan-T5	99	0.010
CNN	BART	3	0.001
	Flan-T5	77	0.001
XSUM	BART	4	0.100
	Flan-T5	98	0.100

Table 3: Fine-Tuning Parameters for Various Tasks

B Dataset Details

Licenses The FLORES, SQUAD, and HotpotQA datasets were used under the Creative Commons Attribution Share Alike 4.0 license; DebateSumm, XSUM, and Reddit-TiFu used the MIT license, the CNN DailyMail dataset used Apache2.0, and WMT17 did not provide a license on the Hugging-Face platform.

Data Splits For training and inference efficiency, we only use subsets of the datasets in some cases. The scripts used to generate the datasets are provided in the repository. At a high level, we take and shuffle the original dataset, then generate a train and test split from that. We perform inference on the test set, for which we report the statistics in the results section. Note that because we employ early stopping, the full training set is not necessarily provided. The number of steps actually taken are reported in Appendix A.

C Analysis of Additional Baselines

In addition to the baselines from previous literature, we compare our method to two baselines that can

Dataset	Train	Val	Test
FLORES Filipino	900	97	1012
WMT DE-EN	2000	100	1000
WMT RU-EN HotpotQA SQUAD	20000	100	1000
	89447	100	1000
	87599	100	1000
DebateSumm Reddit	5000	100	1000
CNN	2000	100	1000
XSUM	20000	100	1000

Table 4: Data Splits by Task

be viewed as straightforward methods of creating a confidence score, namely beam-level entropy (Eq 6) and the sum of the top-k beam probabilities (Eq 7), and report the results in Table 5.

Overall, we find that the performance of the tail method is similar to that of beam-level entropy, although the original tail method performs slightly better in multiple cases.

As for the Top-K baseline, both our ratio and tail methods outperform it on translation and QA tasks for BART, and on QA, English-Russian, DebateSumm, and XSum for T5. However, it underperforms top-K on other tasks, particularly in summarization, which is similar to our findings for the WTP method presented in the main paper.

$$p(\hat{y}^{(i)}) = \sum_{t=1}^{|\hat{y}^{(i)}|} p(\hat{y}_{t}^{(i)}|\hat{y}_{< t}^{(i)}, x)$$

$$p_{\text{Softmax}}(\hat{y}^{(i)}) = \frac{\exp(p(\hat{y}^{(i)}))}{\sum_{j=1}^{k} \exp(p(\hat{y}^{(j)}))}$$

$$\text{Conf}_{\text{Beam Entropy}} = -\sum_{i=1}^{k} p_{\text{softmax}}(\hat{y}^{(i)}) \ln(p_{\text{softmax}}(\hat{y}^{(i)})) \qquad (6)$$

$$\text{Conf}_{\text{Top K Probs}} = \sum_{i=1}^{k} p(\hat{y}^{(i)}) \qquad (7)$$

D Failure Case Examples

We provide examples of cases where there is miscalibration, either due to actual model miscalibration (Table 6), or due to issues with the evaluation strategy (Table 7).

			Fil-EN		DE-EN		RU-EN		HotpotQA		SQUAD		Debate		Reddit		CNN		XSUM	
		Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	Bt	FT5	
Ours		0.649 0.546		0.648 0.653	0.190 0.209	0.779 0.768	0.506 0.491		0.451 0.360	0.494 0.505			0.354 0.293			0.100 0.103				
Base	Entropy Sum Top K			0.648 0.165														0.135 0.120		

Table 5: Spearman correlation (absolute value) between confidence score and evaluation metric/quality score (BLEU for translation, F1 for QA, RougeL for summarization); Bt: BART, FT5: Flan-T5

Overconfident Model: Wrong Translation									
Source: Translate English to Filipino: In the archipelagos and lakes you do not necessarily need a yacht									
Prediction: Ang mga archipelago at mga lupa ay hindi nangangailangan ng isang yacht. (Archipelagos and land do not need a yacht)									
Target: Sa mga arkipelago at mga lawa ay hindi mo naman palaging kakailanganin ang yate. (In archipelagos and lakes, you do not always need a yacht.)									
Overconfident Model: Wrong Translation									
Source: Translate English to Filipino: Scotturb Bus 403 travels regularly to Sintra, stopping at Cabo da Roca									
Prediction: Ang Scotturb Bus 403 ay nagsimula sa Sintra, na nagsimula sa Cabo da Roca. (The Scotturb Bus 403 starts from Sintra, and starts from Cabo de Roca)									

Target: Regular na bumibiyahe ang Scotturb Bus 403 patungong Sintra, tumitigil sa Cabo da Roca. (The Scotturb Bus 403 regularly travels to Sintra, stopping at Cabo da Roca)

Table 6: Examples of outputs where the confidence scores themselves are miscalibrated, taken from the FLORES (Filipino) Dataset (NLLB, 2022)

Good Output Rated as Bad: Correct Gist, Different Style

Source: Manchester United winger Ashley Young celebrated his prominent role in his side's derby win by laughing at 'noisy neighbours' City. The 29-year-old, who scored United's first goal, and created two more for Marouane Fellaini and Chris Smalling, said Louis van Gaal's side were focused on quieting the Manchester City fans... 'Confidence has been sky high for a long time and we want to keep the momentum going now. ... I think it was over when it went to 3-1

Prediction: Ashley Young celebrated his prominent role in his side's derby win by laughing at 'noisy neighbours' City fans. The 29-year-old, who scored United's first goal, and created two more for Marouane Fellaini and Chris Smalling, said Louis van Gaal's side were focused on quieting the Manchester City fans.

Target: Ashley Young scored Manchester United equaliser in 4-2 win. 'We quietened them down straight away' claims Young, as he praises fans. Young claims the game was over once United went 3-1 ahead. England winger says confidence at Old Trafford is now 'sky high'. CLICK HERE to read Ian Ladyman's match report from Old Trafford. READ: Man Utd runaway league leaders in table vs the current top seven

Good Output Rated as Bad: Noisy Label

Source: My first trip to New York was with my aunt when I was about 18 and I had been appearing in Coronation Street for about 12 months... we went to see the musical Chicago on Broadway and did lots and lots of shopping... one of the first things my boyfriend Sylvain Longchambon and I did on my latest trip was to visit the site of the World Trade Center to see the monument to those who died... Coronation Street star Samia Ghadie and boyfriend Sylvain Longchambon take a selfie in New York... The JW Marriott Essex House as seen from Central Park, of which it boasts panoramic views... On the second night of our break, we went on the Bateaux New York cruise, which offers an unforgettable three-hour trip along the Hudson River... The couple, who met as partners on Dancing on Ice, enjoyed a Bateaux New York Cruise of the Hudson... We were wondering who was going to emerge when out stepped Lady Gaga. It was the ultimate holiday treat - it was just a shame I couldn't arrange a selfie with her. That would have been the icing on the cake. American Sky (0843 636 2001) offers a three-night holiday to New York from £899pp. This includes accommodation in the JW Marriott Essex House New York on a room-only basis and return flights with British Airways from Heathrow. Visit nycgo com for more information

Prediction: My first trip to New York was with my aunt when I was about 18 and I had been appearing in Coronation Street for about 12 months. We had a lot of fun together - we went to see the musical Chicago on Broadway and did lots and lots of shopping. We returned to the city that never sleeps in January 2001, eight months before the terrible events of 9/11, and one of the first things my boyfriend Sylvain Longchambon and I did on my latest trip was to visit the site of the World Trade Center to see the monument to those who died.

Target: Samia Ghadie and boyfriend Sylvain Longchambon spent four days in NYC. While there the Dancing on Ice stars stayed at the JW Marriott Essex House. Their suite on the 31st floor offered up panoramic views of Central Park. The couple enjoyed a three-hour Bateaux New York cruise on the Hudson. The confirm Burger Joint in Le Parker Meridien Hotel lives up to the hype.

Bad Output Rated as Good: Repeated Phrase

Source: SOURCE: An exotic animal owner from Ohio is campaigning for his bear and big cats to be returned after they were seized by the state in January. In total, six tigers, a bear, a lion, a cougar, a black leopard and a liger (part lion, part tiger) were taken from Kenny Hetrick's Stony Ridge farm after it was found he did not have the correct permit and cages were 'unsafe'. Authorities have also started cracking down on the owners of wild creatures following an incident in 2011 where a man in eastern Ohio released 56 exotic animals - including lions and tigers - then killed himself. Apparently Hetrick has been heartbroken by the clampdown on his farm and the 72-year-old widower is now fighting to overturn the seizure, ... 'He's lost without them,' said Josh Large, who lives four houses away...

Prediction: In total, six tigers, a bear, a lion, a cougar, a black leopard and a liger were taken from Kenny Hetrick's Stony Ridge farm. In total, six tigers, a bear, a lion, a cougar, a black leopard and a liger were taken from Kenny Hetrick's Stony Ridge farm after it was found he did not have the correct permit and cages were 'unsafe'. Authorities have also started cracking down on the owners of wild creatures following an incident in 2011 where a man in eastern Ohio released 56 exotic animals - including lions and tigers - then killed himself. Hetrick has been heartbroken by the clampdown on his farm and the 72-year-old widower is now fighting to overturn the seizure, backed by neighbors who insist his menagerie doesn't pose a threat.

Target: In total, six tigers, a bear, a lion, a cougar, a black leopard and a liger (part lion, part tiger) were taken from Kenny Hetrick's Stony Ridge farm. State officials found he didn't have the right permit and cages were 'unsafe' But now the 72-year-old is fighting to overturn the seizure, backed by neighbors who insist his menagerie doesn't pose a threat. 'He's lost without them,' said Josh Large, who lives four houses away.

Table 7: Examples of outputs where the outputs are rated incorrectly based on the metric, taken from the CNN-DailyMail Dataset (See et al., 2017)