



# Training-Inference Mismatch In LLM KD

Alephia 25/6/25

# BACKGROUND



模型 $q_\theta$ 依据前缀 $w^{t-1}$ 生成文本的时候，loss可以表示为

$$l(q_\theta, w^{t-1}; o) = \mathbb{E}_{w_t \sim o(\cdot|w^{t-1})} \log \frac{o(w_t|w^{t-1})}{q_\theta(w_t|w^{t-1})}$$

由目标分布 $o$ 采样下一个token  $w_t$ ，再进行KLD对齐。

可以展开得到

$$L(q_\theta; o) \approx \sum_{t=1}^T \mathbb{E}_{w^{t-1} \sim d_o^{t-1}, w_t \sim o(\cdot|w^{t-1})} \log \frac{o(w_t|w^{t-1})}{q_\theta(w_t|w^{t-1})}$$



# TRAIN-INFERENCE MISMATCH

由于模型能力不足，生成token的分布与目标分布存在差距，进而模型训练和推理时面对的前缀是不同的

- Distribution Mismatch (Exposure Bias)
- Error Accumulation

Distribution Mismatch会导致Error Accumulation，且Accumulation行为无法被已有的loss捕捉

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Arora, K., Asri, L.E., Bahuleyan, H., & Cheung, J.C. Why Exposure Bias Matters: An Imitation Learning Perspective of Error Accumulation in Language Generation. In ACL, 22

# TRAIN-INFERENCE MISMATCH



模型与目标的总偏差表示为

$$\begin{aligned} L(q_\theta; o) &= \sum_{t=1}^T \mathbb{E}_{w^{t-1} \sim d_o^{t-1}, w_t \sim o(\cdot|w^{t-1})} \log \frac{o(w_t|w^{t-1})}{q_\theta(w_t|w^{t-1})} \\ &= \sum_{t=1}^T \mathbb{E}_{w^{t-1} \sim d_o^{t-1}} D_{KL}(o(\cdot|w^{t-1}) || q_\theta(\cdot|w^{t-1})) \end{aligned}$$

记生成第 $t$ 个token的期望误差为

$$\epsilon_t = \mathbb{E}_{w_0^{t-1} \sim d_o^t, w_t \sim o(\cdot|w^{t-1})} \log \frac{o(w_t|w^{t-1})}{q_\theta(w_t|w^{t-1})}$$

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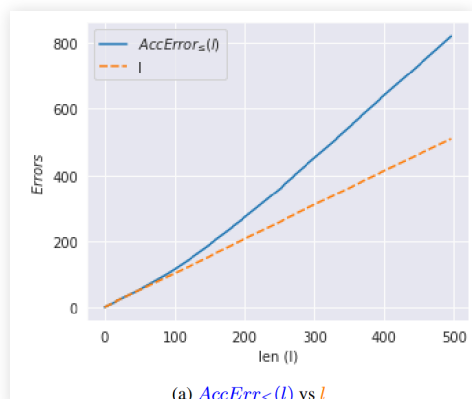
Arora, K., Asri, L.E., Bahuleyan, H., & Cheung, J.C. Why Exposure Bias Matters: An Imitation Learning Perspective of Error Accumulation in Language Generation. In ACL, 22

# TRAIN-INFERENCE MISMATCH

$$l\epsilon_{\leq l} \leq L_{\leq l}(q_\theta) \leq l^2\epsilon_{\leq l}, \quad \epsilon_{\leq l} = \frac{1}{l} \sum_{t=1}^l \epsilon_t$$

$$AccErr_{\leq}(l) = \frac{L_{\leq l}(q_\theta)}{\epsilon_{\leq l}}$$

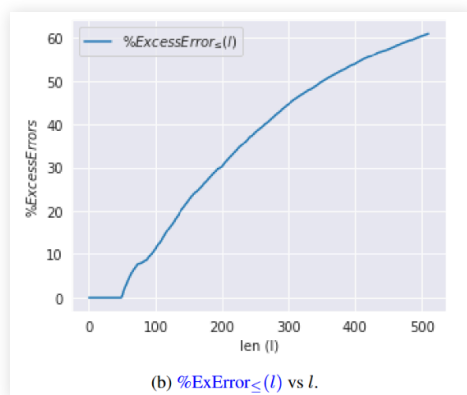
如果Distribution Mismatch确实会导致误差累积的话，应当观察到AccErr值是随着序列长度增加而超线性增长的。



# TRAIN-INFERENCE MISMATCH

$$ExAccErr_{\leq}(l) = \frac{L_{\leq l}(q_{\theta}) - l\epsilon_{\leq l}}{l\epsilon_{\leq l}} \cdot 100$$

如果一个模型能够做到每一个的损失不会累积的话，那么这个值应当一直在0左右，否则，就会呈不断上升的趋势。





# TRAIN-INFERENCE MISMATCH

$$\begin{aligned}\epsilon &= \frac{1}{T} \sum_{t=1}^T \mathbb{E}_{w_0^{t-1} \sim d_o^t} \mathbb{E}_{w_t \sim o(\cdot | w_0^{t-1})} \log \frac{o(w_t | w_0^{t-1})}{q_\theta(w_t | w_0^{t-1})} \\ &\approx -\frac{1}{|D|} \sum_{(w_0^{i-1}, w_i) \in D} \log q_\theta(w_i | w_0^{i-1}) + c \\ &= H(q_\theta; D) + c'\end{aligned}$$

这里 $H(q_\theta; D)$ 代表log Perplexity

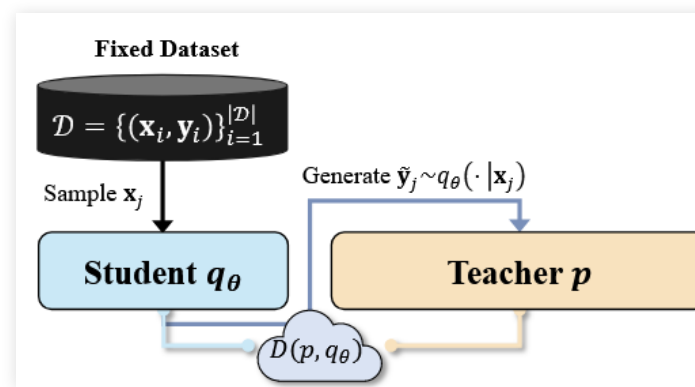
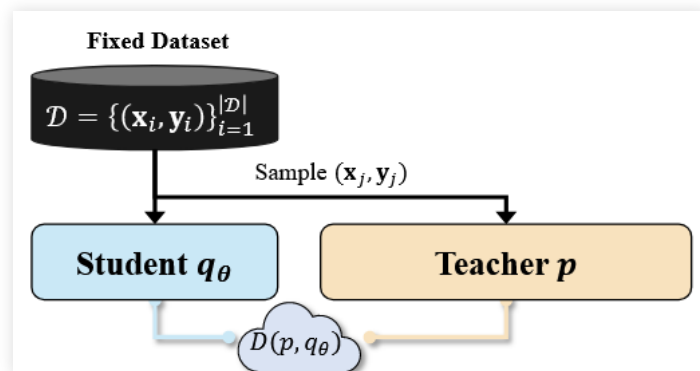
不管是CE Loss，还是Perplexity，都无法监督error的累加过程

# THE UTILIZATION OF SGO

引入模型自己推理生成的内容用于训练(Student Generated Output)

$$L_{SGO}(q_{\theta}; o) = \sum_{t=1}^T \mathbb{E}_{w^{t-1} \sim d_{q_{\theta}}^{t-1}, w_t \sim o(\cdot | w^{t-1})} \log \frac{o(w_t | w^{t-1})}{q_{\theta}(w_t | w^{t-1})}$$

每次有 $\lambda$ 的概率使用SGO， $1 - \lambda$ 的概率使用训练集样本



Agarwal, R., Vieillard, N., Zhou, Y., Stańczyk, P., Ramos, S., Geist, M., & Bachem, O. On-Policy Distillation of Language Models: Learning from Self-Generated Mistakes. In ICLR, 24



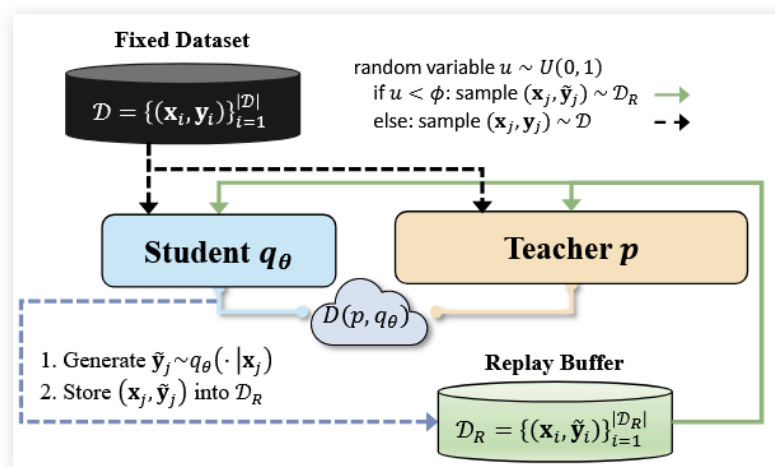
# THE UTILIZATION OF SGO

- 使用SGO时, Teacher也面临Train-Inference Mismatch, 会带来噪声

💡 更加保守地使用SGO

- 每次都要学生重新生成SGO, 利用率低, 计算开销大

💡 on-policy  $\rightarrow$  off-policy



Ko, J., Kim, S., Chen, T., & Yun, S. DistiLLM: Towards Streamlined Distillation for Large Language Models. In ICML, 24

# THE UTILIZATION OF SGO

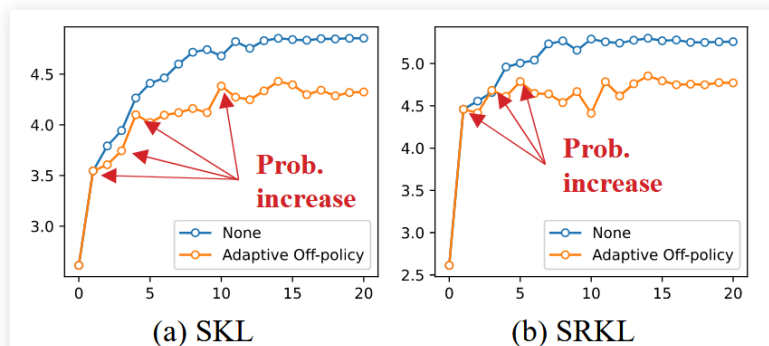


Figure 10. Plot of validation loss values (y-axis) across each validation iteration (x-axis). Although validation loss tends to increase as training progresses, employing SGO effectively prevents this increase. This is the core philosophy of our adaptive SGO scheduler (orange line).

Loss  $\uparrow$ , ROUGE\_L  $\uparrow$

"Our observations indicate that training on a diverse range of SGOs, rather than solely on a fixed dataset, mitigates training-inference mismatch and consequently lowers validation loss"

过拟合? train-inference mismatch? 指标与loss的不匹配?



# INTRODUCE SAMPLE-WISE WEIGHT

$P$ 为真实分布， $Q$ 为合成数据分布， $q_\theta$ 为模型预测分布

$$E_Q[-\log q_\theta(y|x; \theta)]$$

$$E_Q \left[ -\frac{P(y|x)}{Q(y|x)} \log q_\theta(y|x; \theta) \right] = E_P[-\log q_\theta(y|x; \theta)]$$

$P(y|x)$ 大，数据点与真实分布高度相关且明确，有参考意义。  
 $Q(y|x)$ 越小，数据点在分布 $Q$ 中所包含的信息越多。

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Kuo, H., Liao, Y., Chao, Y., Ma, W., & Cheng, P. Not All LLM-Generated Data Are Equal: Rethinking Data Weighting in Text Classification. In ICLR, 25



# INTRODUCE SAMPLE-WISE WEIGHT

加权策略更新为

$$E_Q \left[ - \frac{q_{\theta}(y|x; \theta, D_{P'})}{q_{\theta}(y|x; \theta)} \log q_{\theta}(y|x; \theta) \right]$$

$q_{\theta}(y|x)$  越小，模型在这个数据点上学的越差，越应注重

Dataset	Method	Financial		Tweet Irony		MRPC	
		Acc	F1	Acc	F1	Acc	F1
Small real world	GPT-3.5 few-shot	79.46	81.6	63.39	69.39	69.28	71.75
	CE-Loss (quality checker)	78.05	75.26	62.5	62.38	73.16	68.69
	Focal-Loss	78.47	76.2	67.73	62.32	73.10	66.64
	DIMP-Loss (Ours)	<b>79.87</b>	<b>77.05</b>	<b>69.01</b>	<b>67.05</b>	<b>74.84</b>	<b>66.80</b>
GPT-3.5 generated	CE-Loss	77.39	74.01	76.91	76.8	72	65.47
	Focal-Loss	79.29	75.32	74.87	74.82	72.17	62.77
	Hu et al.'s	71.7	61.93	71.42	70.18	67.13	50.08
	SunGen	80.45	76.87	78.96	75.06	71.65	66.08
	IMP-Loss (Ours)	82.09	<b>79.40</b>	<b>81.89</b>	<b>81.71</b>	<b>75.83</b>	<b>70.52</b>
	DIMP-Loss (Ours)	<b>82.67</b>	<b>79.53</b>	78.44	78.14	<b>75.83</b>	<b>70.04</b>
	- w/o diversity checker	81.35	77.94	77.68	77.62	74.72	69.34
Large real world	CE-Loss	84.74	82.69	68.75	68.41	80.92	77.73
	Focal-Loss	<b>84.98</b>	81.98	67.6	67.19	80.35	76.28
	Hu et al.'s	80.19	76.58	60.33	37.63	71.36	67.78
	SunGen	84.65	82.51	63.9	62.66	80.81	78.78
	IMP-Loss (Ours)	<b>85.3</b>	<b>83.27</b>	<b>70.15</b>	<b>70.08</b>	81.33	78.3
	DIMP-Loss (Ours)	<b>85.4</b>	<b>82.79</b>	69	68.78	<b>82.84</b>	<b>80.49</b>

# THINKINGS



🤔 Add weight to SGO ?

$$L_{WSGO}(q_{\theta}; o) = \sum_{t=1}^T \mathbb{E}_{w^{t-1} \sim d_o^{t-1}} \lambda(t-1, w^{t-1}) D_{KL}(o(\cdot|w^{t-1}) || q_{\theta}(\cdot|w^{t-1}))$$

🤔 When using SGO, add adaptive weight for  $L_{Base}$  w.r.t  $L_{KD}$  ?

$$L = L_{KD} + \phi_{epoch} L_{Base}$$

🤔 Deeper research in teacher's response to SGO ?

🤔 How to solve error accumulation?

# LLM KD WITH DIFFERENT VOCABULARIES



教师( $m \times D$ )向学生( $n \times d$ )对齐:

$$Q = P^q([e_{1:n}^s; e_{2:n+1}^s]; \theta_P^q) \in R^{n \times 2D}$$

$$K = [e_{1:m}^t; e_{2:m+1}^t] \in R^{m \times 2D}$$

$$V = P^v(e_{2:m+1}^t + h_{1:m}^t; \theta_P^v) \in R^{m \times d}$$

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Zhang, S., Zhang, X., Sun, Z., Chen, Y., & Xu, J. Dual-Space Knowledge Distillation for Large Language Models. In EMNLP, 24

# LLM KD WITH DIFFERENT VOCABULARIES



教师变换后的emd可以表示为

$$h_{1:n}^{t \rightarrow s} = \text{softmax}\left(\frac{QK^T}{\sqrt{2D}}V\right) \in R^{n \times d}$$

最后过学生的映射头得到概率分布

$$p^t = \text{softmax}(h_{1:n}^{t \rightarrow s} \mathbf{W}_S)$$

# THANKS!

