Method	Single-Document QA	Multi-Document QA	Summarization	Few-shot Learning	Synthetic	
	MF-zh	DuReader	VCSum	LSHT	PR-zh	Avg. ↑
Avg len	6,701	15,768	15,380	22,337	6,745	
		Qwen2-7B-Instruct,	KV Size = Full			
FullKV	39.17	23.63	16.21	43.50	70.50	38.60
	Qwenz	2-7B-Instruct, KV Size (	Compression Ratio	0 = 10%		
StreamingLLM	38.05	23.24	15.92	40.50	44.50	32.44
H2O	37.99	19.58	16.16	41.67	67.35	36.55
SnapKV	44.25	20.27	16.24	44.50	68.10	38.67
PyramidKV	36.57	20.56	16.15	43.50	66.50	36.55
ChunkKV	45.92	20.15	16.37	43.75	71.10	39.45

Table 17: Performance comparison of Chinese subtask on LongBench for Qwen2-7B-Instruct.

## C. Theoretical Understanding

In this section, we provide the theoretical interpretation from the perspective from the In-context learning (ICL) to further understand how ChunkKV outperforms token-level KV cache compression.

**Pretraining Data Distribution.** Given a set of concepts  $\Theta$  and a concept  $\theta \in \Theta$ , we define the pretraining data is sampled from  $p(o_1, \ldots, o_T) = \int_{\theta \in \Theta} p(o_1, \ldots, o_T | \theta) p(\theta) d\theta$  (Fang & Xie, 2022). Each token o is sampled from a vocabulary  $\mathbb O$ . For simplicity, we write  $o_{1:t} = o_1 \ldots o_t$ .

**Language Modeling.** Current LLMs (Brown et al., 2020; Touvron et al., 2023; Fang & Xie, 2022) usually utilize the next word prediction as the language modelling, which predicts the next token  $o_t$  given the previous tokens  $o_1 \dots o_{t-1}$  for all  $t=1,\dots,T$ . Formally, a language modelling can be writen as the distribution  $f(o_t|o_{1:t-1})$ . And it is pretrained on a huge corpus sampled from the pretraining distribution  $p(o_1,\dots,o_{t+1})$  (Fang & Xie, 2022). Considering the large scale of the model size and dataset size, it can be assumed that the  $f(o_1 \dots o_{t+1})$  has been aligned with the  $p(o_1 \dots o_{t+1})$  (Fang & Xie, 2022).

**Prompt Distribution.** Following (Fang & Xie, 2022), a prompt is composed of an input token sequence x followed by an output token y. Then, the i-th training example  $^1$  that can appear in any place in the whole prompt  $o_{1:T}$  is defined as  $O_i$  consisting of an input  $x_i = O_i [1:k-1]$  (the first k-1 tokens) followed by the output  $y_i = O_i [k]$  at the end, where the length k is fixed for simplicity.

The *i*-th training example is independently generated as follows: 1) Generate a start hidden state  $h_i^{\text{start}}$  from a *prompt* start distribution  $p_{\text{prompt}}$ ; 2) Given  $h_i^{\text{start}}$ , generate the example sequence  $O_i = [x_i, y_i]$  from  $p(O_i | h_i^{\text{start}}, \theta^*)$ . The test input  $x_{\text{test}} = x_{n+1}$  is sampled similarly. Then, the prompt consists of a sequence of training examples  $(S_n)$  followed by the example  $x_{\text{test}}$ :

$$[S_n, x_{\text{test}}] = [x_1, y_1, x_2, y_2, \dots, x_n, y_n, x_{\text{test}}] \sim p_{\text{prompt}}.$$
 (2)

**In-context learning setups and Assumptions.** We follow other settings and assumptions in (Fang & Xie, 2022). With the greedy decoding (Fu et al., 2024b), sampling the next token from the language modeling  $f(o_t|o_{1:t-1})$  becomes the predictor as  $y = \arg\max_{o_t} f(o_t|o_{1:t-1})$ .

Thus, for  $[S_n, x_{\text{test}}]$ , the in-context learning predictor can be written as  $f_n(x_{\text{test}}) := \arg\max_y p(y|S_n, x_{\text{test}})$ , which outputs the most likely prediction over the *pretraining distribution* conditioned on the *prompt distribution*. Its expected 0-1 error with n examples is  $L_{0-1}(f_n) = \mathbb{E}_{x_{\text{test}}, y_{\text{test}} \sim p_{\text{prompt}}}[\mathbf{1}[f_n(x_{\text{test}}) \neq y_{\text{test}}]]$ .

We define  $p_{\theta}^{i}(o) := p(O[i] = o|O[1:i-1], \theta)$  of the i-th token with previous tokens and the analogous distribution  $p_{prompt}^{i} := p_{prompt}(O[i] = o|O[1:i-1])$  under the prompt distribution. Following (Fang & Xie, 2022), there is a distinguishability condition formalizes when in-context learning occurs giving the concept  $\theta$ .

The distinguishability condition is dependent on a KL divergence between the previous two distributions and the error terms

<sup>&</sup>lt;sup>1</sup>Here, training example in prompts means happens during the prompt learning.