Neural Knowledge Bank for Pretrained Transformers

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Abstract

The ability of pretrained Transformers to remember factual knowledge is essential but still limited for existing models. Inspired by existing work that regards Feed-Forward Networks (FFNs) in Transformers as key-value memories, we design a Neural Knowledge Bank (NKB) and a knowledge injection strategy to introduce extra factual knowledge for pretrained Transformers. The NKB is in the form of additional knowledgeable memory slots to the FFN and the memory-like architecture makes it highly interpretable and flexible. When injecting extra knowledge with the Salient Span Masking (SSM) pretraining objective, we fix the original pretrained model and train only the NKB. This training strategy makes sure the general language modeling ability of the original pretrained model is not influenced. By mounting the NKB onto the T5 model, we verify its strong ability to store extra factual knowledge based on three closed-book question answering datasets. Also, we prove that mounting the NKB will not degrade the general language modeling ability of T5 through two representative tasks, summarization and machine translation. Further, we thoroughly analyze the interpretability of the NKB and reveal the meaning of its keys and values in a human-readable way. Finally, we show the flexibility of the NKB by directly modifying its value vectors to update the factual knowledge stored in it.

1 Introduction

In recent years, large-scale pretrained Transformers (Devlin et al. 2019; Liu et al. 2019; Dong et al. 2019; Clark et al. 2020; Raffel et al. 2020) have contributed greatly to natural language processing. They are usually trained on large-scale corpora, which contain oceans of factual knowledge. When facing some knowledge-intensive downstream tasks such as closed-book question answering, the ability to remember factual knowledge will be especially essential. Petroni et al. (2019) show that pretrained Transformers can recall some factual knowledge that appears in the training corpus in a zero-shot manner. Roberts, Raffel, and Shazeer (2020) also prove that after fine-tuning, T5 (Raffel et al. 2020) can answer some open-domain questions without access to external knowledgeable contexts. Even so, the ability of pretrained models to store factual knowledge is still limited (Porner, Walttinger, and Schütze 2019; Cao et al. 2021).

Considering this actuality, in this paper, we aim to design an interpretable method to introduce extra factual knowledge for pretrained Transformers. Geva et al. (2020) point out that Feed-Forward Networks (FFNs) in Transformers work in a similar way to key-value memories. As shown in Figure 1, in an FFN, we regard the first linear layer as a set of keys and the second linear layer as the corresponding values. The input hidden state of the FFN is fed into the first linear layer and activates a set of intermediate neurons. Then, taking these activated neurons as weights, the second linear layer integrates the corresponding value vectors through weighted sum. On top of this view, Dai et al. (2022) further find that FFNs in pretrained Transformers store factual knowledge in a memory-like manner.

Inspired by the above findings, we design a Neural Knowledge Bank (NKB) and a knowledge injection strategy to introduce extra factual knowledge for pretrained Transformers. The NKB is an FFN-like module concatenated after the FFN as additional knowledgeable memory slots. In order to inject factual knowledge, we first acquire...
a knowledgeable corpus from Wikipedia and then pretrain the NKB with the Salient Span Masking (SSM) (Guo et al. 2020) pretraining objective. Note that during knowledge injection, we fix the original pretrained model to avoid influencing its general language modeling ability. For downstream tasks, we can directly fine-tune the whole model. The advantages of the NKB are reflected in three aspects: (1) The knowledge injection process for the NKB is independent of the original pretrained model, so introducing extra knowledge will not degrade the general language modeling ability of the original model. (2) The memory-like architecture of the NKB makes it highly interpretable and we can explain the meaning of its keys and values in a human-readable way. (3) The key-value architecture of the NKB has high flexibility and we can easily perform knowledge updating on the NKB by modifying its value vectors.

On three closed-book question answering datasets in different domains, we find that mounting the NKB can boost the performance of T5, especially in the biomedical domain that the T5 pretraining corpus does not cover much. Also, through two representative tasks, summarization and machine translation, we prove that mounting the NKB will not degrade the general language modeling ability of the original T5 model. Further, we thoroughly analyze the NKB to reveal its working mechanism and present the meaning of its keys and values in a human-readable way. Finally, we show the flexibility of the NKB by directly modifying its value vectors to update the factual knowledge stored in it.

Our contributions are summarized as follows:

- We propose the idea of the NKB, including its architecture and knowledge injection strategy, to neurally store extra factual knowledge for pretrained Transformers.
- We verify that the NKB can boost the performance of T5 on closed-book question answering and meanwhile keep its general language modeling ability.
- We analyze the interpretability of the NKB and reveal the meaning of its keys and values in a human-readable way.
- We show the flexibility of the NKB by directly modifying its value vectors to update the factual knowledge in it.

### 2 Background: Transformer

Recently, Transformer (Vaswani et al. 2017) has been the most popular and effective architecture in natural language processing. Taking a standard Transformer encoder as an example, it is stacked with \( \ell \) identical Transformer layers. In each Transformer layer, there are two main modules: a self-attention (SelfAtt) module and a feed-forward network (FFN). For an input sequence with \( \text{len} \) tokens, let \( X \in \mathbb{R}^{\text{len} \times d} \) denote the input hidden states of a Transformer layer, we formulate these two modules as follows:

\[
Q_h = X W^Q_h, \quad K_h = X W^K_h, \quad V_h = X W^V_h, \quad \text{SelfAtt}_h(X) = \text{Softmax}(Q_h K_h^T) V_h, \quad \text{FFN}(H) = \text{ActFunc}(HW^T_1) W_2, \quad \text{where } W^Q_h, W^K_h, W^V_h \in \mathbb{R}^{d \times \frac{d}{\text{head}}}, W_1, W_2 \in \mathbb{R}^{4d \times d} \text{ are parameter matrices}, \text{SelfAtt}_h(X) \text{ computes the } h\text{-th of the } n \text{ attention heads, } H \in \mathbb{R}^{\text{len} \times d} \text{ denotes the output hidden states of the self-attention module, which is computed by projecting the concatenation of all the attention heads, and } \text{ActFunc} \text{ denotes the activation function such as GELU (Hendrycks and Gimpel 2016) or ReLU (Glorot, Bordes, and Bengio 2011). We omit the scaling factor in the self-attention module and the bias terms for simplicity.}
\]

Comparing Equation (2) and Equation (3), we can find that the calculation formula of FFN\((\cdot)\) is almost the same as that of SelfAtt\(_h(\cdot)\), except that they have different non-linear functions. Therefore, it is reasonable to view the FFN as a module with the query-key-value mechanism. Specifically, the FFN input \( H \) serves as queries, the parameters of the first linear layer \( W_1 \) are keys, and the parameters of the second linear layer \( W_2 \) are values. This view of the FFN is also supported by Geva et al. (2020, 2022), Dai et al. (2022).

### 3 Method

Following Geva et al. (2020, 2022), Dai et al. (2022), we also view FFNs in Transformer as key-value memories. On top of this view, we design a Neural Knowledge Bank (NKB) and a knowledge injection strategy to introduce extra factual knowledge for pretrained Transformers. In this section, we introduce the view of the FFN as key-value memory, the architecture of the NKB, and the knowledge injection method.

#### 3.1 Key-value Memory View of FFN

We first formulate the FFN as key-value memory like Geva et al. (2020), Dai et al. (2022). As illustrated in Figure 1, we regard the input hidden state \( h \in \mathbb{R}^d \) of a token as a query, and the parameter matrices \( W_1, W_2 \in \mathbb{R}^{4d \times d} \) of two linear layers as \( 4d \) keys and \( 4d \) values, respectively, where each key or value is a \( d \)-dimension vector. First, \( h \) is fed into the first linear layer. For each key vector in \( W_1 \), we compute a scalar score \( s_i \) through inner product:

\[
s_i = h^T W_1[i, :], \quad (4)
\]

where \([\cdot, \cdot]\) denotes the slice operation for a matrix. Then, after activation, these scores compose the intermediate hidden state \( \text{h}^{(\text{inter})} \in \mathbb{R}^{4d} \) of the FFN:

\[
w_i = \text{ActFunc}(s_i), \quad (5)
\]

\[
\text{h}^{(\text{inter})} = [w_1; w_2; \ldots; w_{4d}], \quad (6)
\]

where \([\cdot; \cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\·
Transformer layer, we allocate two new matrices $W'_1, W'_2 \in \mathbb{R}^{d' \times d'}$ as additional keys and values, where $d'$ is a hyperparameter that control the capacity of the NKB. As illustrated in Figure 2, we mount the NKB onto a Transformer layer by concatenating $W'_1$ and $W'_2$ after $W_1$ and $W_2$ in the original FFN, respectively.

With the NKB, the intermediate hidden state $h^{(\text{inter})}$ of the FFN will be extended to $(4d + d')$-dimensions:

$$s'_i = h^T W'_1 [i, :], \quad w'_i = \text{ActFunc}(s'_i),$$

$$h^{(\text{inter})}_{i} = [w_1; w_2; \ldots; w_{4d}; w'_1; w'_2; \ldots; w'_{d'}],$$

where $w'_i$ is the weight of the $i$-th additional memory slot. Finally, taking the new $h^{(\text{inter})}$ as weights, the value vectors in $W_2$ and $W'_2$ are integrated as follows:

$$h^{(\text{output})} = \sum_{i=1}^{4d} w_i W_2[i, :) + \sum_{i=1}^{d'} w'_i W'_2[i, :].$$

Also, we omit the bias terms in the above formulations.

As a simple extension of the FFN, the NKB is easy to implement and use. More importantly, the memory-like architecture of the NKB makes it highly interpretable and we can explain the meaning of its keys and values in a human-readable way. Also, the key-value architecture has high flexibility and we can easily perform knowledge updating on the NKB by directly modifying its value vectors.

3.3 Knowledge Injection

In order to introduce extra factual knowledge, we pretrain the NKB with the Salient Span Masking (SSM) (Guu et al. 2020; Roberts, Raffel, and Shazeer 2020) pretraining objective. To be specific, we first acquire a knowledgeable corpus (i.e., named entities and dates) in each text segment using the entity recognizer in spaCy. We randomly mask one of the salient spans and train the parameters of the NKB to reconstruct the masked salient span.

Note that during knowledge injection, we freeze the parameters in the original pretrained model and update only the parameters in the NKB. Compared with previous work (Roberts, Raffel, and Shazeer 2020) that updates the pretrained parameters for knowledge injection, our training strategy can avoid the general language modeling ability of the pretrained model being degraded due to parameter changes. In addition, with this training strategy, new factual knowledge is precisely injected into the NKB, so it also becomes easier to locate and analyze the newly introduced factual knowledge. After knowledge injection, we can directly fine-tune the whole model for downstream tasks.

4 Experiments

4.1 Tasks

Following Roberts, Raffel, and Shazeer (2020), we use the closed-book question answering task to evaluate the factual knowledge stored in the parameters of a model. Compared with open-domain question answering (Prager 2006) that requires the model to answer context-independent questions about facts in the real world, the closed-book setting has a more strict constraint that the model cannot access external resources when answering questions. Therefore, a model can address closed-book question answering well only if it can store the factual knowledge in its pretrained parameters.

In addition, in order to evaluate the general language modeling ability of a model, we also consider two representative tasks, summarization and machine translation. They are not heavily dependent on external factual knowledge and can evaluate whether a model can model and generate languages.

4.2 Datasets

For closed-book question answering, we use three datasets in this paper: two general-domain datasets, Natural Questions (Kwiatkowski et al. 2019) and WebQuestions (Be-
We use AdaFactor (Shazeer and Stern 2018) as the optimizer and do not apply dropout for the NKB. We list the complete hyper-parameters for three datasets in Appendix A due to the space limit.

For downstream tasks, we fine-tune all the parameters in $T_5\text{base}+\text{NKB}$. We tune the hyper-parameters on the validation set and report the best validation performance for each dataset. For closed-book question answering, following (Roberts, Raffel, and Shazeer 2020), we use AdaFactor (Shazeer and Stern 2018) as the optimizer. For summarization and machine translation, we use AdamW (Loshchilov and Hutter 2017) as the optimizer. The complete hyper-parameters are different for each dataset, so we list them in Appendix B due to the space limit.

### 4.4 Baselines

In order to show the advantages of the NKB, we compare $T_5\text{base}+\text{NKB}$ with four baselines: (1) Transformer denotes a vanilla Transformer model that shares the same architecture with $T_5\text{base}$, but its parameters are randomly initialized without pretraining. (2) $T_5\text{base}$ and $T_5\text{large}$ denote the standard T5 pretrained models with 220M and 770M parameters, respectively. (3) $T_5\text{base}+\text{NKB}$ denotes a model that shares the same architecture with $T_5\text{base}+\text{NKB}$ but all its parameters are updated during knowledge injection.

### 4.5 Results

#### Closed-book Question Answering

The results on closed-book question answering are shown in Table 3. We use the Exact Match (EM) score as the metric, which evaluates whether the generated answer is totally the same as one of the ground-truth answers. From the table, we have the following observations: (1) The vanilla Transformer without pretraining performs extremely poorly on closed-book question answering since it is not knowledgeable at all. (2) With pretraining, $T_5\text{base}$ achieves a good EM score on the general-domain datasets (i.e., Natural Questions and WebQuestions), but on the biomedical-domain dataset HEAD-QA, it also performs poorly since biomedical texts account for only a small proportion in the T5 pretraining corpus. (3) With more parameters, $T_5\text{large}$ achieves better performance than $T_5\text{base}$, but it still cannot address the biomedical-domain closed-book question answering well. (4) With only 5M more parameters, the NKB significantly boosts the performance of $T_5\text{base}$, which approaches the performance of $T_5\text{large}$ on the general-domain datasets and largely outperforms $T_5\text{large}$ on the biomedical-domain dataset. (5) On closed-book question answering, knowledge injection for only 5M parameters in the NKB ($T_5\text{base}+\text{NKB}$) can achieve a comparable performance with $T_5\text{base}+\text{NKB}$-a that updates all the parameters during knowledge injection.

#### Summarization and Machine Translation

Ideal knowledge injection should inject new factual knowledge into a pretrained model but not negatively influence the general language modeling ability of the original model. We use summarization and machine translation, two representative tasks that do not heavily rely on external factual knowledge to evaluate the general language modeling ability of models.
| Model       | # Params | # Knowledgeable Params | Natural Questions | WebQuestions | HEAD-QA | Average |
|-------------|----------|------------------------|-------------------|--------------|---------|---------|
| Transformer | 220M     | N/A                    | 0.4               | 2.0          | 0.2     | 0.9     |
| T5<sub>base</sub> | 220M | N/A                    | 26.3              | 29.9         | 3.7     | 20.0    |
| T5<sub>base</sub>+NKB-a | 225M | 225M                   | 26.9              | **31.9**     | **11.0** | **23.3** |
| T5<sub>base</sub>+NKB | 225M | 5M                     | **27.4**          | 31.1         | **11.0** | **23.2** |
| T5<sub>large</sub> | 770M | N/A                    | 28.5              | 31.5         | 5.0     | 21.7    |

Table 3: Exact Match (EM) scores on closed-book question answering. # Knowledgeable Params denote the parameters that are trained during knowledge injection. With 5M more parameters, the NKB boosts the performance of T5<sub>base</sub> by 3.2 EM scores on average, exceeding the performance of T5<sub>large</sub> with 3.4 times of parameters. We also find that during knowledge injection, training only the NKB (T5<sub>base</sub>+NKB) can achieve a comparable performance with training all the parameters (T5<sub>base</sub>+NKB-a).

| Model       | Xsum (Rouge-L) | WMT-En-De (BLEU) | WMT-En-Ro (BLEU) | Average |
|-------------|----------------|------------------|------------------|---------|
| Transformer | 20.7           | 21.5             | 21.9             | 21.4    |
| T5<sub>base</sub> | 30.1 | **30.5**         | 28.2             | **29.6** |
| T5<sub>base</sub>+NKB-a | 24.9 | 25.9             | 25.1             | 25.3    |
| T5<sub>base</sub>+NKB | 30.1 | **30.5**         | 28.2             | **29.6** |

Table 4: Results on summarization and machine translation. Training all the parameters (T5<sub>base</sub>+NKB-a) during knowledge injection introduces a negative impact on the performance of T5<sub>base</sub> for these two tasks. By contrast, training only the NKB (T5<sub>base</sub>+NKB) will not degrade the general language modeling ability of T5<sub>base</sub>.

### 5 Interpretability of NKB

#### 5.1 Value Vectors Store Entities

Dai et al. (2022) find that FFNs can store factual knowledge, and more specifically, Geva et al. (2022) state that the value vectors in FFNs are often corresponding to human-readable concepts. Inspired by them, we analyze the NKB value vectors in the output vocabulary space and find that most of the value vectors store specific entities.

**Method**

We randomly sample NKB value vectors from the best T5<sub>base</sub>+NKB checkpoint fine-tuned on WebQuestions for analysis. For the i-th value vector \(v_i \in \mathbb{R}^d\), we first project it into the output vocabulary space and get a probability distribution \(p_i \in \mathbb{R}^{N_{vocab}}\) over the output vocabulary:

\[
p_i = \text{Softmax}(Ev_i),
\]

where \(E \in \mathbb{R}^{N_{vocab} \times d}\) is the output embedding matrix in T5<sub>base</sub>. Then, for each sampled value vector \(v_i\), we manually check the token that has the highest probability in \(p_i\) and classify it into one out of six entity categories: Person, Place, Organization, Date, Other, or Non-entity. In order to guarantee the confidence of the manual annotation, we ignore tokens that are not complete words or not in English. Finally, we annotate 100 valid value vectors.

**Results**

For each entity category, we show an example value vector and its top-scoring token in Table 5. We also present the distribution of all the top-scoring tokens over the entity categories in Figure 3. We find that 85% of the sampled value vectors are corresponding to specific entities. The entity information in the value vectors will be integrated into the FFN output hidden state \(h_{\text{output}}\) and contribute to the generation of the final answer.

#### 5.2 Entity Category Vectors

We use Rouge-L (Lin 2004) as the metric for summarization and SacreBLEU (Post 2018) for machine translation. We demonstrate the results in Table 4, where the NKB is trained on the WebQuestions-related knowledgeable corpus. We have the following findings: (1) With pretraining, T5<sub>base</sub> achieves much better performance than the vanilla Transformer on all the datasets. (2) Although performing well on closed-book question answering, T5<sub>base</sub>+NKB-a has a poor performance on summarization and machine translation since it changes the pretrained parameters of T5<sub>base</sub> during knowledge injection. (3) For T5<sub>base</sub>+NKB, we train only the newly introduced parameters, so the general language modeling ability of T5<sub>base</sub> will not be negatively influenced. As a result, T5<sub>base</sub>+NKB can not only address knowledge-intensive tasks like closed-book question answering well, but also keep a good performance on other tasks that do not heavily rely on external factual knowledge.

| Value | Top-scoring Token | Entity Category |
|-------|-------------------|-----------------|
| v71   | Norway            | Place           |
| v2878 | Constantin        | Organization    |
| v2170 | Columbus          | Person          |
| v221  | 1974              | Date            |
| v1581 | Portuguese        | Other           |
| v1046 | desert            | Non-entity      |

Table 5: Example NKB value vectors and their top-scoring tokens with the highest probability.
Table 6: Example NKB key vectors and their top-triggering questions. We can identify a common and human-readable semantic pattern among the top-triggering questions for 78% of the sampled key vectors.

| Key  | Top-triggering Questions                                                                 | Common Semantic Pattern               |
|------|-----------------------------------------------------------------------------------------|---------------------------------------|
| k_{726} | What kind of language do Egyptians speak?  
What was the ancient Egyptians’ spoken language?  
What language is mainly spoken in Egypt? | Ask about the language of Egypt         |
| k_{1452} | What school did Mark Zuckerberg attend?  
What college did Albert Einstein go to?  
What university did Obama graduate from? | Ask about the schools of celebrities   |
| k_{2750} | What style of art did Henri Matisse do?  
What type of artist is Henri Matisse?  
What genre of art is the Mona Lisa? | Ask about the art genre                |

Figure 3: Distribution of the top-scoring tokens for 100 sampled NKB value vectors. 85% of the sampled value vectors are corresponding to specific entities.

5.2 Key Vectors Capture Input Patterns
Compared with the NKB value vectors that store input-independent entities, the NKB key vectors are input-sensitive. They are responsible for determining when to activate the memory slots according to the input patterns. In this section, by analyzing when the memory slots are activated, we reveal the patterns that trigger the key vectors.

**Method** We analyze the same T5_{base}+NKB checkpoint used in Section 5.1. To be specific, we input each question in the validation set of WebQuestions into the model. When the model is generating the first answer token for a question, we record its NKB weights (i.e., the intermediate hidden state in the NKB). After the NKB weights for all the questions are recorded, we randomly sample 100 key vectors for analysis. For the i-th key vector k_i \in \mathbb{R}^d, we select out 5 questions that trigger the key vector the most (i.e., have the highest NKB weights). Finally, we manually check these 5 questions and attempt to identify human-readable semantic patterns that appear in at least 2 questions.

**Results** From the manual annotation, we find that 78% of the sampled keys have common semantic patterns in their top-triggering questions. We show some example key vectors and their top-triggering questions in Table 6 for a better understanding of the patterns. Putting the findings about the NKB keys and values together, we can summarize the working mechanism of the NKB as follows: the key vectors determine whether to activate the memory slots according to the input patterns, and then the value vectors of the activated memory slots are integrated to contribute to generating the final answer entity.

6 Knowledge Updating for NKB
The knowledge updating ability for a model is meaningful to avoid the model producing erroneous or outdated results. Taking advantage of the flexible key-value architecture of the NKB, we propose a simple method to directly update the answer of a question to another one by performing a small knowledge surgery on the NKB.

**Data** We select examples from the validation set of WebQuestions for knowledge updating. In order to guarantee the validity of the target answer, we select the questions for which the model predicts wrong answers, and aim to update these wrong answers to correct ones. In this paper, we only consider the questions that have single-token ground-truth answers and predicted answers. Finally, we keep 67 examples for the following knowledge updating experiments.

**Method** Inspired by Dai et al. (2022), we perform a small knowledge surgery on the NKB to eliminate the information of the original answer and introduce new information of the target answer. To be specific, for a question, we first select the memory slot with the highest NKB weight. Then, we perform the following operation on the NKB:

\[ v_t \leftarrow \lambda (e_{tgt} - e_{ori}), \]

where t is the index of the highest-weight memory slot, \( \lambda \) is a hyper-parameter, \( e_{ori} \) and \( e_{tgt} \) denote the output word embeddings of the original answer and the target answer, respectively. Intuitively, by modifying only one value vector (accounting for only 0.00034% of the whole model parameters), the knowledge surgery tends to suppress the predicted probability of the original answer and encourage the model to generate the target answer.
some factual knowledge but to a limited extent, so enhancing pretrained models with extra knowledge is still meaningful.

### Enhancing Pretrained Models with External Knowledge

Recently, many efforts have been paid to incorporate external knowledge for pretrained models. ERNIE (Zhang et al. 2019) and KnowBERT (Peters et al. 2019) enhance the word representations with external knowledge graphs during pretraining or continual pretraining. KEPLER (Wang et al. 2021b) optimizes the objectives of masked language modeling and knowledge embedding jointly on the same pretrained model. K-adapter (Wang et al. 2021a) injects two kinds of knowledge into specific adapters in series while keeping the original pretrained model fixed. K-BERT (Liu et al. 2020) appends relevant triplets to the input sentence to enhance sentence encoding during fine-tuning. Kformer (Yao et al. 2022) retrieves relevant knowledgeable texts during fine-tuning and encodes them into dense vectors to extend the FFN. Our NKB combines the advantages of the existing methods: it injects extra knowledge before fine-tuning, can keep the modeling ability of the original pretrained model, and more importantly, is highly interpretable.

### Understanding FFNs in Transformers

Recently, the Feed-Forward Networks (FFNs), which account for about two-thirds of the parameters in a Transformer, have been proved especially important (Wu et al. 2019, Dong, Cordonnier, and Loukas 2021) to Transformers. Geva et al. (2020) build a connection between FFNs and key-value memories. Geva et al. (2022) further regard the value vectors in FFNs as sub-updates that encode human-readable concepts. Dai et al. (2022) point out that FFNs store factual knowledge in a memory-like manner, and the knowledge neurons in FFNs are positively correlated to the expression of their corresponding facts. Inspired by them, we propose the FFN-like NKB to introduce extra factual knowledge for pretrained Transformers in an interpretable way.

### 8 Conclusion

In this paper, we propose a Neural Knowledge Bank (NKB) and a knowledge injection strategy to introduce extra factual knowledge for pretrained Transformers in a neural way. On the closed-book question answering task, we verify that the NKB can store extra factual knowledge and thus boost the performance of the T5 model. Also, we use two representative tasks to prove that mounting the NKB will not degrade the general language modeling ability of the original pretrained model. Further, we show the interpretability of the NKB by revealing its working mechanism and presenting the meaning of its keys and values in a human-readable manner.
way. Finally, we show the flexibility of the NKB by directly modifying its value vectors to update the factual knowledge stored in it. Considering the cost of experiments, we only evaluate and analyze the NKB based on T5 in this paper, but the NKB is also applicable to other pretrained models based on the Transformer architecture.

References

Berant, J.; Chou, A.; Frostig, R.; and Liang, P. 2013. Semantic Parsing on Freebase from Question-Answer Pairs. In EMNLP 2013, 1533–1544.

Cao, B.; Lin, H.; Han, X.; Sun, L.; Yan, L.; Liao, M.; Xue, T.; and Xu, J. 2021. Knowledgeable or Educated Guess? Re-visiting Language Models as Knowledge Bases. In ACL-IJCNLP 2021, 1860–1874.

Chen, D.; Fisch, A.; Weston, J.; and Bordes, A. 2017. Reading Wikipedia to Answer Open-Domain Questions. In ACL 2017, 1870–1879.

Clark, K.; Luong, M.; Le, Q. V.; and Manning, C. D. 2020. ELECTRA: Pre-training Text Encoders as Discriminators Rather Than Generators. In ICLR 2020. OpenReview.net.

Dai, D.; Dong, L.; Hao, Y.; Sui, Z.; Chang, B.; and Wei, F. 2022. Knowledge Neurons in Pretrained Transformers. In ACL 2022, 8493–8502.

Devlin, J.; Chang, M.; Lee, K.; and Toutanova, K. 2019. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. In NAACL-HLT 2019, 4171–4186. Association for Computational Linguistics.

Dong, L.; Yang, N.; Wang, W.; Wei, F.; Liu, X.; Wang, Y.; Gao, J.; Zhou, M.; and Hon, H. 2019. Unified Language Model Pre-training for Natural Language Understanding and Generation. In NeurIPS 2019, 13042–13054.

Dong, Y.; Cordonnier, J.; and Loukas, A. 2021. Attention is Not All You Need: Pure Attention Loses Rank Doubly Exponentially with Depth. CoRR, abs/2103.03404.

Elazar, Y.; Kassner, N.; Ravfogel, S.; Ravichander, A.; Hovy, E. H.; Schütze, H.; and Goldberg, Y. 2021. Measuring and Improving Consistency in Pretrained Language Models. CoRR, abs/2102.01017.

Geva, M.; Caciu laru, A.; Wang, K. R.; and Goldberg, Y. 2022. Transformer Feed-Forward Layers Build Predictions by Promoting Concepts in the Vocabulary Space. CoRR, abs/2203.14680.

Geva, M.; Schuster, R.; Berant, J.; and Levy, O. 2020. Transformer Feed-Forward Layers Are Key-Value Memories. CoRR, abs/2012.14913.

Gl orot, X.; Bordes, A.; and Bengio, Y. 2011. Deep Sparse Rectifier Neural Networks. In AISTATS 2011, volume 15 of JMLR Proceedings, 315–323. JMLR.org.

Guu, K.; Lee, K.; Tung, Z.; Pasupat, P.; and Chang, M. 2020. REALM: Retrieval-Augmented Language Model Pre-Training. CoRR, abs/2002.08909.

Hendrycks, D.; and Gimpel, K. 2016. Gaussian Error Linear Units (GELUs). arXiv:1606.08415.
Prager, J. M. 2006. Open-Domain Question-Answering. *Found. Trends Inf. Retr.*, 1(2): 91–231.

Raffel, C.; Shazeer, N.; Roberts, A.; Lee, K.; Narang, S.; Matena, M.; Zhou, Y.; Li, W.; and Liu, P. J. 2020. Exploring the Limits of Transfer Learning with a Unified Text-to-Text Transformer. *Journal of Machine Learning Research*, 21(140): 1–67.

Roberts, A.; Raffel, C.; and Shazeer, N. 2020. How Much Knowledge Can You Pack Into the Parameters of a Language Model? In *EMNLP 2020*, 5418–5426. Association for Computational Linguistics.

Shazeer, N.; and Stern, M. 2018. Adafactor: Adaptive Learning Rates with Sublinear Memory Cost. In *ICML 2018*, 4603–4611.

Vaswani, A.; Shazeer, N.; Parmar, N.; Uszkoreit, J.; Jones, L.; Gomez, A. N.; Kaiser, L.; and Polosukhin, I. 2017. Attention is All you Need. In *NeurIPS 2017*, 5998–6008.

Vilares, D.; and Gómez-Rodríguez, C. 2019. HEAD-QA: A Healthcare Dataset for Complex Reasoning. In *ACL 2019*, 960–966.

Wang, R.; Tang, D.; Duan, N.; Wei, Z.; Huang, X.; Ji, J.; Cao, G.; Jiang, D.; and Zhou, M. 2021a. K-Adapter: Infusing Knowledge into Pre-Trained Models with Adapters. In *ACL-IJCNLP 2021*, volume ACL/IJCNLP 2021 of *Findings of ACL*, 1405–1418. Association for Computational Linguistics.

Wang, X.; Gao, T.; Zhu, Z.; Zhang, Z.; Liu, Z.; Li, J.; and Tang, J. 2021b. KEPLER: A Unified Model for Knowledge Embedding and Pre-trained Language Representation. *Trans. Assoc. Comput. Linguistics*, 9: 176–194.

Wu, F.; Fan, A.; Baevski, A.; Dauphin, Y. N.; and Auli, M. 2019. Pay Less Attention with Lightweight and Dynamic Convolutions. In *7th International Conference on Learning Representations, ICLR 2019*. OpenReview.net.

Yao, Y.; Huang, S.; Zhang, N.; Dong, L.; Wei, F.; and Chen, H. 2022. Kformer: Knowledge Injection in Transformer Feed-Forward Layers. *CoRR*, abs/2201.05742.

Zhang, Z.; Han, X.; Liu, Z.; Jiang, X.; Sun, M.; and Liu, Q. 2019. ERNIE: Enhanced Language Representation with Informative Entities. In *ACL 2019*, 1441–1451. Association for Computational Linguistics.
Appendix

A Hyper-parameters for Knowledge Injection

The hyper-parameters for knowledge injection for three closed-book question answering datasets are summarized in Table 9. We train fewer steps for HEAD-QA since the size of its retrieved knowledgeable corpus is relatively small.

B Hyper-parameters for Fine-tuning

The hyper-parameters for closed-book question answering are summarized in Table 10. For all the reported models, we use the same hyper-parameters.

The hyper-parameters for summarization and machine translation are summarized in Table 11. For all the reported models except for the vanilla Transformer, we use the same hyper-parameters. For the vanilla Transformer, we train 200K steps for summarization and machine translation since it converges more slowly than pretrained models.
| Hyper-parameters | Natural Questions | WebQuestions | HEAD-QA |
|------------------|------------------|-------------|---------|
| # NKB Slot       | 3072             | 3072        | 3072    |
| NKB Position     | the last decoder layer | the last decoder layer | the last decoder layer |
| Dropout for NKB  | 0                | 0           | 0       |
| Sequence Length  | 512 tokens       | 512 tokens  | 512 tokens |
| Batch Size       | 256              | 256         | 256     |
| Dropout          | 0                | 0           | 0       |
| Sequence Length  | 512 tokens       | 512 tokens  | 512 tokens |
| Batch Size       | 256              | 256         | 256     |
| Dropout          | 0                | 0           | 0       |
| Sequence Length  | 512 tokens       | 512 tokens  | 512 tokens |
| Batch Size       | 256              | 256         | 256     |
| Dropout          | 0                | 0           | 0       |
| Sequence Length  | 512 tokens       | 512 tokens  | 512 tokens |
| Batch Size       | 256              | 256         | 256     |
| Dropout          | 0                | 0           | 0       |

Table 9: Hyper-parameters for knowledge injection for three closed-book question answering datasets.

| Hyper-parameters | Natural Questions | WebQuestions | HEAD-QA |
|------------------|------------------|-------------|---------|
| Maximum Sequence Length | 256 tokens     | 256 tokens  | 256 tokens |
| Batch Size       | 768              | 256         | 256     |
| Dropout          | 0                | 0           | 0       |
| Sequence Length  | 512 tokens       | 512 tokens  | 512 tokens |
| Batch Size       | 256              | 256         | 256     |
| Dropout          | 0                | 0           | 0       |
| Sequence Length  | 512 tokens       | 512 tokens  | 512 tokens |
| Batch Size       | 256              | 256         | 256     |
| Dropout          | 0                | 0           | 0       |
| Sequence Length  | 512 tokens       | 512 tokens  | 512 tokens |
| Batch Size       | 256              | 256         | 256     |
| Dropout          | 0                | 0           | 0       |

Table 10: Hyper-parameters for fine-tuning on closed-book question answering.

| Hyper-parameters | Xsum | WMT-En-De | WMT-En-Ro |
|------------------|------|-----------|-----------|
| Maximum Source Sequence Length | 512 tokens | 128 tokens | 128 tokens |
| Maximum Target Sequence Length | 128 tokens | 128 tokens | 128 tokens |
| Batch Size       | 16   | 96        | 96        |
| Dropout          | 0.1  | 0.2       | 0.2       |
| Dropout for NKB  | 0    | 0         | 0         |
| Random Seed      | 1234 | 1234      | 1234      |
| Gradient Clip Norm | 1.0  | 1.0       | 1.0       |
| Label Smoothing  | 0.1  | 0.1       | 0.1       |
| Beam Size        | 4    | 4         | 4         |
| Dropout          | 0.1  | 0.1       | 0.1       |
| Dropout for NKB  | 0    | 0         | 0         |
| Random Seed      | 1234 | 1234      | 1234      |

Table 11: Hyper-parameters for fine-tuning on summarization and machine translation.