

Universal Transformers

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Abstract

Self-attentive feed-forward sequence models have been shown to achieve impressive results on sequence modeling tasks including machine translation [31], image generation [30] and constituency parsing [18], thereby presenting a compelling alternative to recurrent neural networks (RNNs) which has remained the de-facto standard architecture for many sequence modeling problems to date. Despite these successes, however, feed-forward sequence models like the Transformer [31] fail to generalize in many tasks that recurrent models handle with ease (e.g. copying strings or even simple logical inference when the string or formula lengths exceed those observed at training time [28]). **Moreover, and in contrast to RNNs, the Transformer model is not computationally universal, limiting its theoretical expressivity.** In this paper we propose the Universal Transformer which addresses these practical and theoretical shortcomings and we show that it leads to improved performance on several tasks. Instead of recurring over the individual symbols of sequences like RNNs, **the Universal Transformer repeatedly revises its representations of all symbols in the sequence with each recurrent step.** In order to combine information from different parts of a sequence, it employs a self-attention mechanism in every recurrent step. Assuming sufficient memory, its recurrence makes the Universal Transformer computationally universal. We further employ an **adaptive computation time (ACT) mechanism to allow the model to dynamically adjust the number of times the representation of each position in a sequence is revised.** Beyond saving computation, we show that **ACT can improve the accuracy of the model.** Our experiments show that on various algorithmic tasks and a diverse set of large-scale language understanding tasks the Universal Transformer generalizes significantly better and outperforms both a vanilla Transformer and an LSTM in machine translation, and achieves a new state of the art on the bAbI linguistic reasoning task and the challenging LAMBADA language modeling task.

与RNN比较而言，Transformer不能通用，受限于它的理论基础

通用tf重复修改每一个循环步中序列所有标记的表达

self_attention机制
adaptive computation time机制
模型可以动态调整序列中修改表达的次数

ACT可以提高模型精确度

通用tf比LSTM和vanilla tf表现更好

1 Introduction

卷积核全注意力前馈架构的模型应运而生，可以作为RNN的替代品,在处理序列任务上

Convolutional and fully-attentional feed-forward architectures like the Transformer model have recently emerged as viable alternatives to recurrent neural networks (RNNs) for a range of sequence modeling tasks, notably machine translation [9, 31]. These architectures address a significant shortcoming of RNNs, namely their inherently sequential computation which prevents parallelization across elements of the input sequence, whilst still addressing the vanishing gradients problem [15]. The Transformer model in particular achieves this by relying entirely on a self-attention mechanism [22, 19] to compute a series of context-informed vector-space representations of the symbols in

RNN缺点：1.顺序性计算，不能够使输入序列并行化
2.梯度消失和梯度爆炸问题

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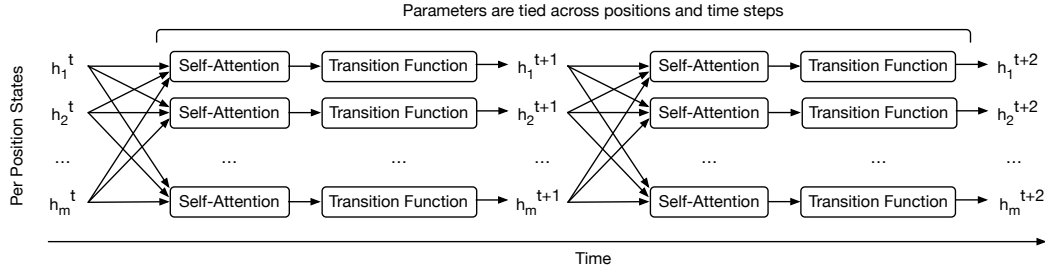


Figure 1: The Universal Transformer repeatedly refines a series of vector representations for each position of the sequence in parallel, by combining information from different positions using self-attention and applying a recurrent transition function. We show this process over two recurrent time-steps. **Arrows denote dependencies between operations.** Initially, h^0 is initialized with the embedding for each symbol in the sequence. h_i^t represents the representation for input symbol $1 \leq i \leq m$ at recurrent time-step t .

箭头表示两种操作的依赖关系
初始化: h^0 =序列中每个标记的词嵌入
 h_i^t 代表在循环时间步 t 时刻的输入标记 $1 \leq i \leq m$

tf模型依赖于自我注意力机制, 计算输入和输出序列的向量, 这些向量用来预测哪些用于结果序列标记, 哪些用于后续的标记分布
这种机制不仅可以直接并行化, 而且由于每个符号的表示也直接由其他所有符号的表示所决定, 这就产生了一个有效的全局接受域。
这与卷积形成对比, 卷积建构有局限的感受野。

its input and output, which are then used to predict distributions over subsequent symbols as the model predicts the output sequence symbol-by-symbol. Not only is this mechanism straightforward to parallelize, but as each symbol's representation is also directly informed by all other symbols' representations, this results in an effectively global receptive field. This stands in contrast to e.g. convolutional architectures which typically have a limited **receptive field**. 感受野

Notably, however, the Transformer foregoes the RNN's inductive bias towards learning iterative or recursive transformations. Our experiments indicate that this inductive bias may be crucial for several algorithmic and language understanding tasks of varying complexity: in contrast to models such as the Neural Turing Machine [13], the Neural GPU [17] or Stack RNNs [16], the Transformer does not generalize well to input lengths not encountered during training.

In this paper, we propose the *Universal Transformer*. It combines the parallelizability and global receptive field of the Transformer model with the recurrent inductive bias of RNNs which seems to be better suited to a range of algorithmic and natural language understanding sequence-to-sequence problems. As the name implies, in contrast to the standard Transformer, under certain assumptions the Universal Transformer can be shown to be computationally universal (Section 4).

In each step, the Universal Transformer iteratively refines its representations for all positions in the sequence in parallel with a self-attention mechanism [22, 19], followed by a recurrent transformation consisting of a depth-wise separable convolution [5] or a position-wise fully-connected layer (see Fig 1). We also extend the Universal Transformer by employing an adaptive computation time mechanism at each position in the sequence [12], allowing the model to choose the required number of refinement steps for each symbol dynamically.

When running for a fixed number of steps, the Universal Transformer is equivalent to a multi-layer Transformer with tied parameters across its layers. However, another, and possibly more informative, way of characterizing the Universal Transformer is as a recurrent function evolving per-symbol hidden states in parallel, based at each step on the sequence of previous hidden states. In this way, it is similar to architectures such as the Neural GPU [17] and the Neural Turing Machine [13]. The Universal Transformer thereby retains the attractive computational efficiency of the original feed-forward Transformer model, but with the added recurrent inductive bias of RNNs. In its adaptive form, we furthermore show that the Universal Transformer can effectively interpolate between the feed-forward, fixed-depth Transformer and a gated, recurrent architecture running for a number of steps dependent on the input data.

Our experimental results show that its recurrence improves results in machine translation, where the Universal Transformer outperforms the standard Transformer with the same number of parameters. In experiments on several algorithmic tasks, the Universal Transformer consistently improves significantly over LSTM RNNs and the standard Transformer. Furthermore, on the bAbI and LAMBADA text understanding data sets, the Universal Transformer achieves a new state of the art.

2 Model

2.1 The Universal Transformer

The Universal Transformer (Fig. 2) is based on the popular encoder-decoder architecture commonly used in most neural sequence-to-sequence models [27, 4, 31]. Both the encoder and decoder of the Universal Transformer operate by applying a recurrent neural network to the representations of each of the positions of the input and output sequence, respectively. However, in contrast to most applications of recurrent neural networks to sequential data, the Universal Transformer does not recur over positions in the sequence, but over consecutive revisions of the vector representations of each position (i.e., over “depth”). In other words, the Universal Transformer is not computationally bound by the number of symbols in the sequence, but only by the number of revisions made to each symbol’s representation.

不受符号数量的限制，仅受修改次数的限制

In each recurrent step, the representation of every position is revised in two sub-steps: first the Universal Transformer uses a self-attention mechanism to exchange information across all positions in the sequence, generating a vector representation for each position that is informed by the representations of all other positions at the previous time-step. Then, it applies a *shared* transition function to the outputs of the self-attention mechanism, independently at each position. Crucially, this is in contrast to most popular neural sequence models, including the Transformer [31] or deep RNNs, which have constant depth by applying a *fixed stack* of layers.

该模型没有固定的深度，transformer和RNN都有固定的深度

For the encoder, given an input sequence of length m , we start with a matrix whose rows are initialized as the d -dimensional embeddings of the symbols at each position of the sequence $H^0 \in \mathbb{R}^{m \times d}$. The Universal Transformer then iteratively computes representations H^t at step t for all m positions in parallel by applying the multiheaded dot-product self-attention mechanism from [31], followed by a recurrent transition function. We also add **residual connections** around each of these function blocks and apply **dropout and layer normalization** [25, 2] (see Fig. 2 for a simplified diagram, and Fig. 4 in the appendix for the complete model.).

transformer中d的大小是key的维度，通过multi-head层和transition-function层

More specifically, our attention mechanism is the scaled dot-product attention

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d}}\right)V \quad (1)$$

transformer中d的大小是key的维度

where d is the number of columns of Q , K and V . We use the multi-head version with k heads, as introduced in [31],

$$\text{MultiHeadSelfAttention}(H) = \text{Concat}(\text{head}_1, \dots, \text{head}_k)W^O \quad (2)$$

$$\text{where head}_i = \text{Attention}(HW_i^Q, HW_i^K, HW_i^V) \quad (3)$$

with affine projections using learned parameter matrices $W^Q \in \mathbb{R}^{d \times d/k}$, $W^K \in \mathbb{R}^{d \times d/k}$, $W^V \in \mathbb{R}^{d \times d/k}$ and $W^O \in \mathbb{R}^{d \times d}$.

At step t , the Universal Transformer computes revised representations $H^t \in \mathbb{R}^{m \times d}$ for all m input positions as follows

$$A^t = \text{LayerNorm}(H^{t-1} + P^t + \text{MultiHeadSelfAttention}(H^{t-1} + P^t))$$

该公式感觉有误

$$\begin{aligned} H^t &= \text{LayerNorm}(A^{t-1} + \text{Transition}(A^t)) \\ \text{where } A^t &= \text{LayerNorm}(H^{t-1} + \text{MultiHeadSelfAttention}(H^{t-1} + P^t)), \end{aligned} \quad (5)$$

$$H^t = \text{LayerNorm}(A^t + \text{Transition}(A^t))$$

where $\text{LayerNorm}()$ is defined in [2], and $\text{Transition}()$ and P^t are discussed below.

Depending on the task, we use one of two different transition functions: either a **separable convolution** [5] or a **fully-connected neural network** that consists of a single rectified-linear **activation function** between two affine transformations, applied position-wise, i.e. individually to each row of A^t .

P^t above are two-dimensional (position, time) *coordinate embeddings*, obtained by computing the sinusoidal position embedding vectors as defined in [31] for the position m and the time-step t

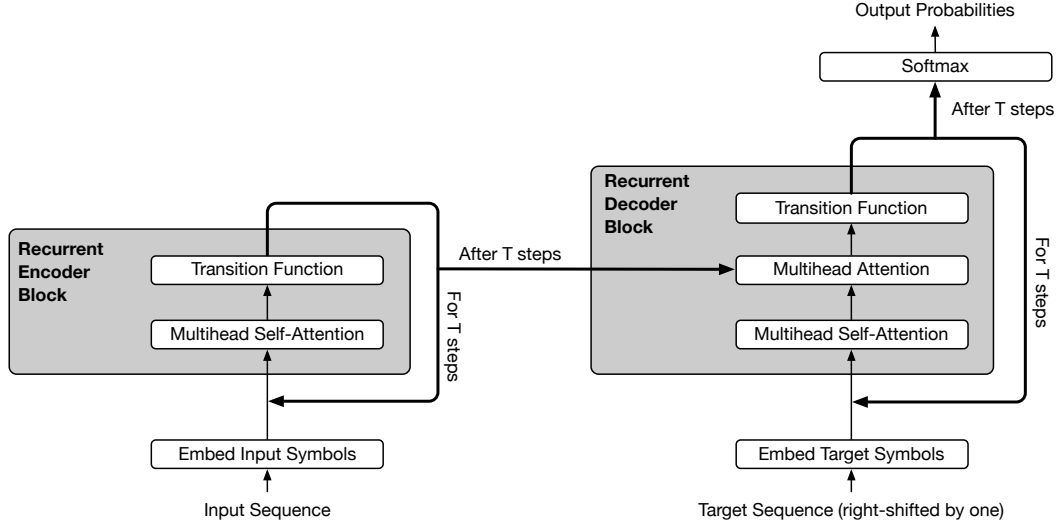


Figure 2: The recurrent blocks of the Universal Transformer encoder and decoder. This diagram omits position and time-step encodings as well as dropout, residual connections and layer normalization. A complete version can be found in the appendix. The Adaptive Universal Transformer dynamically determines the number of steps T for each position using ACT.

separately for each vector-dimension j , and summing these vectors component-wise (denoted by \oplus):

$$\begin{aligned} P_{pos,2j}^t &= \sin(pos/10000^{2j/d}) \oplus \sin(t/10000^{2j/d}) \\ P_{pos,2j+1}^t &= \cos(pos/10000^{2j/d}) \oplus \cos(t/10000^{2j/d}). \end{aligned} \quad (6)$$

修改输入信息

每一步都会平行的修改输入序列中的所有位置

After T steps (each of which refines all positions of the input sequence in parallel), the final output of the Universal Transformer encoder is a matrix of d -dimensional vector representations $H^T \in \mathbb{R}^{m \times d}$ for the m symbols of the input sequence.

decoder和encoder的结构是一样的

The decoder shares the same basic recurrent structure of the encoder. However, after the self-attention function, the decoder additionally also attends to the final encoder representation H^T of each position in the input sequence using the same multihead dot-product attention function from Equation 2, but with queries Q obtained from projecting the decoder representations, and keys and values (K and V) obtained from projecting the encoder representations (this process is akin to standard attention [3]).

这段讲了decoder比encoder多了en-de attention层，Q来自于decoder的self-attention层，KV来自于encoder的输出

Like the Transformer model, the Universal Transformer is autoregressive [11]. Trained using teacher-forcing, at generation time it produces its output one symbol at a time, with the decoder consuming the previously produced output positions. During training, the decoder input is the target output, shifted to the right by one position. The decoder self-attention distributions are further masked such that the model can only attend to positions to the left of any predicted symbol. Finally, the per-symbol target distributions are obtained by applying an affine transformation $O \in \mathbb{R}^{d \times V}$ from the final decoder state to the output vocabulary size V , followed by a softmax which yields an $(m \times V)$ -dimensional output matrix normalized over its rows:

解码器分布self-attention进行了屏蔽，使模型只能从已经预测的符号中获得信息。

$$p(y_{pos} | y_{[1:pos-1]}, H^T) = \text{softmax}(OH^T)^1 \quad (8)$$

To generate from the model, the encoder is run once for the conditioning input sequence. Then the decoder is run repeatedly, consuming all already-generated symbols, while generating one additional distribution over the vocabulary for the symbol at the next output position per iteration. We then typically select the highest probability symbol as the next symbol.

¹Note that T here denotes time-step T and not the transpose operation.

2.2 The Adaptive Universal Transformer ACT : 自适应计算次数

In sequence processing systems, certain symbols (e.g. some words or phonemes) are usually more ambiguous than others. **It is therefore reasonable to allocate more processing resources to these more ambiguous symbols.** Adaptive Computation Time (ACT) [12] is a mechanism for dynamically modulating the number of computational steps needed to process each input symbol in standard recurrent neural networks based on a scalar *pondering* value predicted by the model at each step, reflecting the model’s estimation that further computation is required for that step.

分配更多的计算资源去处理更加模糊的符号

Inspired by the interpretation of Universal Transformers as applying parallel recurrent transformations to all positions in the sequence, we also add a dynamic **ACT halting mechanism** to each position. Once the per-symbol recurrent block halts, its state is simply copied to the next step until all blocks halt, or we reach a maximum number of steps (see Fig. 2, with T dynamically determined for each position). The final output of the encoder is then the final layer of representations produced in this way. We call this dynamically-halting version of our model the *Adaptive Universal Transformer*.

一旦某个符号循环快停止了，它的状态会简单的复制到下一步，直到所有的块都停止，或者达到最大的迭代次数

3 Experiments

In this section, we evaluate the Universal Transformer on a range of algorithmic and language understanding tasks, as well as on machine translation. All code and datasets reproducing these results will be released as open source.

3.1 bAbI Question-Answering

The bAbI question answering dataset [32] consists of 20 different tasks, where the goal is to answer a question given a number of English sentences that encode potentially multiple supporting facts. The goal is to measure various forms of language understanding by requiring a certain type of reasoning over the linguistic facts presented in each story. A standard Transformer does not achieve good results on this task². However, we have designed a model based on the Universal Transformer which achieves state-of-the-art results on this task.

To encode the input, similar to [14], we first encode each fact in the story by applying a learned multiplicative positional mask to each word’s embedding, and summing up all embeddings. We embed the question in the same way, and then feed the (Universal) Transformer with these embeddings of the facts and questions.

As originally proposed, models can either be trained on each task separately (“train single”) or jointly on all tasks (“train joint”). Table 1 summarizes our results. We conducted 10 runs with different initializations and picked the best model based on performance on the validation set, similar to previous work. Both the Adaptive and non-adaptive Universal Transformer achieve state-of-the-art results on all tasks in terms of average error and number of failed tasks³, in both the 10K and 1K training regime (see Appendix for breakdown by task).

To understand the working of the model better, we analyzed both the attention distributions and the average ACT ponder times for this task (see the Appendix for the details). First, we observe that the attention distributions start out very uniform, but get progressively sharper in later steps around the correct supporting facts that are required to answer each question, which is indeed very similar to how humans would solve the task. Second, with ACT we observe that the average ponder time (i.e. depth of the per-symbol recurrent processing chain) for tasks requiring three supporting facts is higher than for tasks requiring only two, which is in turn higher than for tasks requiring only one supporting fact. Finally, we observe that the histogram of ponder times at different positions is more uniform in tasks requiring only one supporting fact compared to two and three, and likewise for tasks requiring two compared to three. Especially for tasks requiring three supporting facts, many positions halt at step 1 or 2 already and only a few get transformed for more steps (see for example Fig 3). This is particularly interesting as the length of stories is indeed much higher in this setting, with more irrelevant facts which the model seems to successfully learn to ignore in this way.

²We experimented with different hyper-parameters and different network sizes, but it always overfits.

³Defined as $> 5\%$ error.

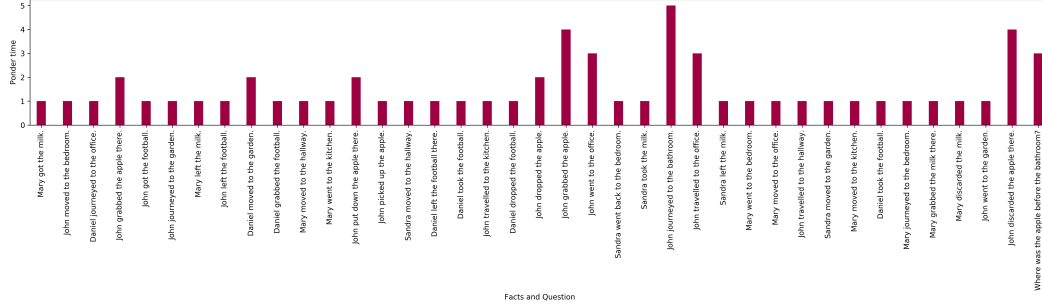


Figure 3: Ponder time of Adaptive Universal Transformer for encoding facts in a story and question in a bAbI task requiring three supporting facts.

Model	10K examples		1K examples	
	train single	train joint	train single	train joint
Previous best results:				
QRNet [24]	0.3 (0/20)	-	-	-
Sparse DNC [23]	-	2.9 (1/20)	-	-
GA+MAGE [8]	-	-	8.7 (5/20)	-
MemN2N [26]	-	-	-	12.4 (11/20)
Our Results:				
Transformer [31]	15.2 (10/20)	22.1 (12/20)	21.8 (5/20)	26.8 (14/20)
Universal Transformer (this work)	0.23 (0/20)	0.47 (0/20)	5.31 (5/20)	8.50 (8/20)
Adapt. Univ. Transformer (this work)	0.21 (0/20)	0.29 (0/20)	4.56 (3/20)	7.85 (5/20)

Table 1: Average error and number of failed tasks ($> 5\%$ error) out of 20 (in parentheses; lower is better in both cases) on the bAbI dataset under the different training/evaluation setups. We indicate state-of-the-art where available for each, or ‘-’ otherwise.

3.2 Subject-Verb Agreement

Next, we consider the task of predicting number agreement between subject and verb in naturally occurring English sentences [20]. This task acts as a proxy for measuring the ability of a model to capture hierarchical (dependency) structure in natural language sentences. We use the dataset provided by [20] and follow their experimental protocol of solving the task using a language modeling training setup, i.e. a next word prediction objective, followed by calculating the ranking accuracy of the target verb at test time. We evaluated our model on subsets of the test data with different task difficulty, measured in terms *agreement attractors* – the number of intervening nouns with the opposite number from the subject. For example, given the sentence *The keys to the cabinet*⁴, the objective during training is to predict the verb *are*. At test time, we then evaluate the ranking accuracy of the correct form of the verb compared to the incorrect form of the verb: i.e. the goal is to rank *are* higher than *is* in this case.

Our results are summarized in Table 2. Best LSTM with attention achieve 99.18% on this task, outperforming a vanilla transformer [28]. The Universal Transformer improves on the Transformer results, and the Adaptive Universal Transformer achieves results comparable to the current state of the art (99.2%).

3.3 LAMBADA Language Modeling

The LAMBADA task [21] is a language modeling task consisting of predicting a missing target word given its (target) sentence and a broader context of 4-5 preceding sentences. The dataset was specifically designed such that humans are able to accurately predict the target word when shown the full context, but not when only shown the target sentence. It therefore goes beyond language modeling, and tests the ability of a model to incorporate broader discourse and longer term context when predicting the target word.

⁴*Cabinet* is an agreement attractor in this case.

Model	Number of attractors						Total
	0	1	2	3	4	5	
Previous best results [33]:							
Best Stack-RNN	0.994	0.979	0.965	0.935	0.916	0.880	0.9923
Best LSTM	0.993	0.972	0.95	0.922	0.900	0.842	0.9911
Best Attention	0.994	0.977	0.959	0.929	0.907	0.842	0.9918
Our results:							
Transformer	0.9733	0.9412	0.9316	0.9167	0.9014	0.8834	0.9616
Universal Transformer	0.9934	0.9712	0.9690	0.9400	0.9206	0.8915	0.9917
Adapt. Univ. Transf. (small)	0.9932	0.9801	0.9714	0.9608	0.9521	0.9314	0.9920
Adapt. Univ. Transf. (base)	0.9943	0.9720	0.9516	0.9567	0.9314	0.9034	0.9924

Table 2: Accuracy on the subject-verb agreement number prediction task (higher is better).

Model	LM Perplexity & (Accuracy)			RC Accuracy		
	control	dev	test	control	dev	test
Neural Cache [10]	129	139	-	-	-	-
Dhingra et al. [7]	-	-	-	-	-	0.5569
Transformer	154 (0.14)	5336 (0.0)	9725 (0.0)	0.4102	0.4401	0.3988
LSTM	138 (0.23)	4966 (0.0)	5174 (0.0)	0.1103	0.2316	0.2007
Universal Transformer	131(0.32)	279 (0.18)	319 (0.17)	0.4801	0.5422	0.5216
Adaptive Universal Transformer	130 (0.32)	135 (0.22)	142 (0.19)	0.4603	0.5831	0.5625

Table 3: LAMBADA language modeling (LM) perplexity (lower better) with accuracy in parentheses (higher better), and Reading Comprehension (RC) accuracy results (higher better). ‘-’ indicates no reported results in that setting.

The task is evaluated in two settings: as *language modeling* (the standard setup) and as *reading comprehension*. In the former (more challenging) case, a model is simply trained for next-word prediction on the training data, and evaluated on the target words at test time (i.e. the model is trained to predict all words, not specifically challenging target words). In the latter setting, introduced by Chu et al. [6], the target sentence (minus the last word) is used as query for selecting the target word from the context sentences. Note that the target word appears in the context 81% of the time, making this setup much simpler. However the task is impossible in the remaining 19% of the cases.

The results are shown in Table 3. Universal Transformer achieves state-of-the-art results in both the language modeling and reading comprehension setup, outperforming both LSTMs and vanilla Transformers. Note that the control set was constructed similar to the LAMBADA development and test sets, but without filtering them in any way, so achieving good results on this set shows a model’s strength in standard language modeling.

3.4 Algorithmic Tasks

We evaluated the Universal Transformer on three algorithmic tasks, namely Copy, Reverse, and (integer) Addition, all on strings composed of decimal symbols (‘0’-‘9’). We train the model using positions starting with randomized offsets to further encourage the model to learn position-relative transformations. Results are shown in Table 4. The Universal Transformer outperforms both LSTM and vanilla Transformer by a wide margin on all three tasks. The Neural GPU reports perfect results on this task [17], however we note that this result required a special curriculum-based training protocol which was not used for other models.

3.5 Learning to Execute (LTE)

As another class of sequence-to-sequence learning problems, we also evaluate Universal Transformers on tasks indicating the ability of a model to learn to execute computer programs, as proposed in [34].

Model	Copy		Reverse		Addition	
	char-acc	seq-acc	char-acc	seq-acc	char-acc	seq-acc
LSTM	0.45	0.09	0.66	0.11	0.08	0.0
Transformer	0.53	0.03	0.13	0.06	0.07	0.0
Universal Transformer	0.91	0.35	0.96	0.46	0.34	0.02
Neural GPU*	1.0	1.0	1.0	1.0	1.0	1.0

Table 4: Accuracy (higher better) on the algorithmic tasks, trained on decimal strings of length 40 and evaluated on length 400 from [17]. *Note that the Neural GPU was trained with a special curriculum to obtain the perfect result, while other models are trained without any curriculum.

Model	Copy		Double		Reverse	
	char-acc	seq-acc	char-acc	seq-acc	char-acc	seq-acc
LSTM	0.78	0.11	0.51	0.047	0.91	0.32
Transformer	0.98	0.63	0.94	0.55	0.81	0.26
Universal Transformer	1.0	1.0	1.0	1.0	1.0	1.0

Table 5: Character-level (*char-acc*) and sequence-level accuracy (*seq-acc*) results on the Memorization LTE tasks, with maximum length of 55.

Model	Program		Control		Addition	
	char-acc	seq-acc	char-acc	seq-acc	char-acc	seq-acc
LSTM	0.53	0.12	0.68	0.21	0.83	0.11
Transformer	0.71	0.29	0.93	0.66	1.0	1.0
Universal Transformer	0.89	0.63	1.0	1.0	1.0	1.0

Table 6: Character-level (*char-acc*) and sequence-level accuracy (*seq-acc*) results on the Program Evaluation LTE tasks with maximum nesting of 2 and length of 5.

Model	BLEU
Universal Transformer <i>small</i>	26.8
Transformer <i>base</i> [31]	28.0
Weighted Transformer <i>base</i> [1]	28.4
Universal Transformer <i>base</i>	28.9

Table 7: Machine translation results on the WMT14 En-De translation task trained on 8xP100 GPUs in comparable training setups. All *base* results have the same number of parameters.

These tasks include program evaluation tasks (program, control, and addition), and memorization tasks (copy, double, and reverse).

We use the mix-strategy discussed in [34] to generate the datasets. Unlike [34], we do not use any curriculum learning strategy during training and we make no use of target sequences at test time. Tables 5 and 6 present the performance of an LSTM model, Transformer, and Universal Transformer on the program evaluation and memorization tasks, respectively. Universal Transformer achieves perfect scores in all the memorization tasks and outperforms both LSTMs and Transformers in all program evaluation tasks.

3.6 Machine Translation

We evaluated on the standard WMT 2014 English-German translation task using the same setup as reported in [31]. Results are summarized in Table 7. The Universal Transformer with a fully-connected recurrent function (instead of separable convolution) and without ACT improves by 0.9 BLEU over a Transformer and 0.5 BLEU over a Weighted Transformer with approximately the same number of parameters [1].

4 Universality and Relationship to Other Models

Given sufficient memory the Universal Transformer is computationally universal – i.e. it belongs to the class of models that can be used to simulate any Turing machine, thereby addressing a shortcoming of the standard Transformer model. Despite being theoretically appealing, our results show that this added expressivity also leads to improved accuracy on several challenging sequence modeling tasks. This closes the gap between practical sequence models competitive on large-scale tasks such as machine translation, and computationally universal models such as the Neural Turing Machine or the Neural GPU [13, 17], which can be trained using gradient descent to perform algorithmic tasks.

To show this, we can reduce a Neural GPU to a Universal Transformer. Ignoring the decoder and parameterizing the self-attention mechanism to be the identity function, we assume the transition function to be a convolution. If we now set the total number of recurrent steps T to be equal to the input length, we obtain exactly a Neural GPU. Note that the last step is where the Universal Transformer crucially differs from the vanilla Transformer whose depth cannot scale dynamically with the size of the input. A similar relationship exists between the Universal Transformer and the Neural Turing Machine, whose single read/write operations per step can be expressed by the global, parallel representation revisions of the Universal Transformer. In contrast to these models, however, which only perform well on algorithmic tasks, the Universal Transformer also achieves competitive results on realistic natural language tasks such as LAMBADA and machine translation.

Another related model architecture is that of end-to-end Memory Networks [26]. In contrast to end-to-end memory networks, however, the Universal Transformer uses memory corresponding to states aligned to individual positions of its inputs or outputs. Furthermore, the Universal Transformer follows the encoder-decoder configuration and achieves competitive performance in large-scale sequence-to-sequence tasks.

5 Conclusion

This paper introduces the Universal Transformer, a generalization of the Transformer model that extends its theoretical capabilities and produces state-of-the-art results on a wide range of challenging sequence modeling tasks, such as language understanding but also a variety of algorithmic tasks, thereby addressing a key shortcoming of the standard Transformer. The Universal Transformer combines the following key properties into one model:

Weight sharing: Following intuitions behind weight sharing found in CNNs and RNNs, we extend the Transformer with a simple form of weight sharing that strikes the right balance between inductive bias and model expressivity, which we show extensively on both small and large-scale experiments.

Conditional computation: In our goal to build a computationally universal machine, we equipped the Universal Transformer with the ability to halt or continue computation through a recently introduced mechanism, which shows stronger results compared to the fixed-depth Universal Transformer.

We are enthusiastic about the recent developments on parallel-in-time sequence models. By adding computational capacity and recurrence in processing depth, we hope that further improvements beyond the basic Universal Transformer presented here will help us build learning algorithms that are both more powerful, data efficient, and generalize beyond the current state-of-the-art.

The code used to train and evaluate Universal Transformers is available at <https://github.com/tensorflow/tensor2tensor> [29].

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Appendix A Detailed Schema of the Universal Transformer

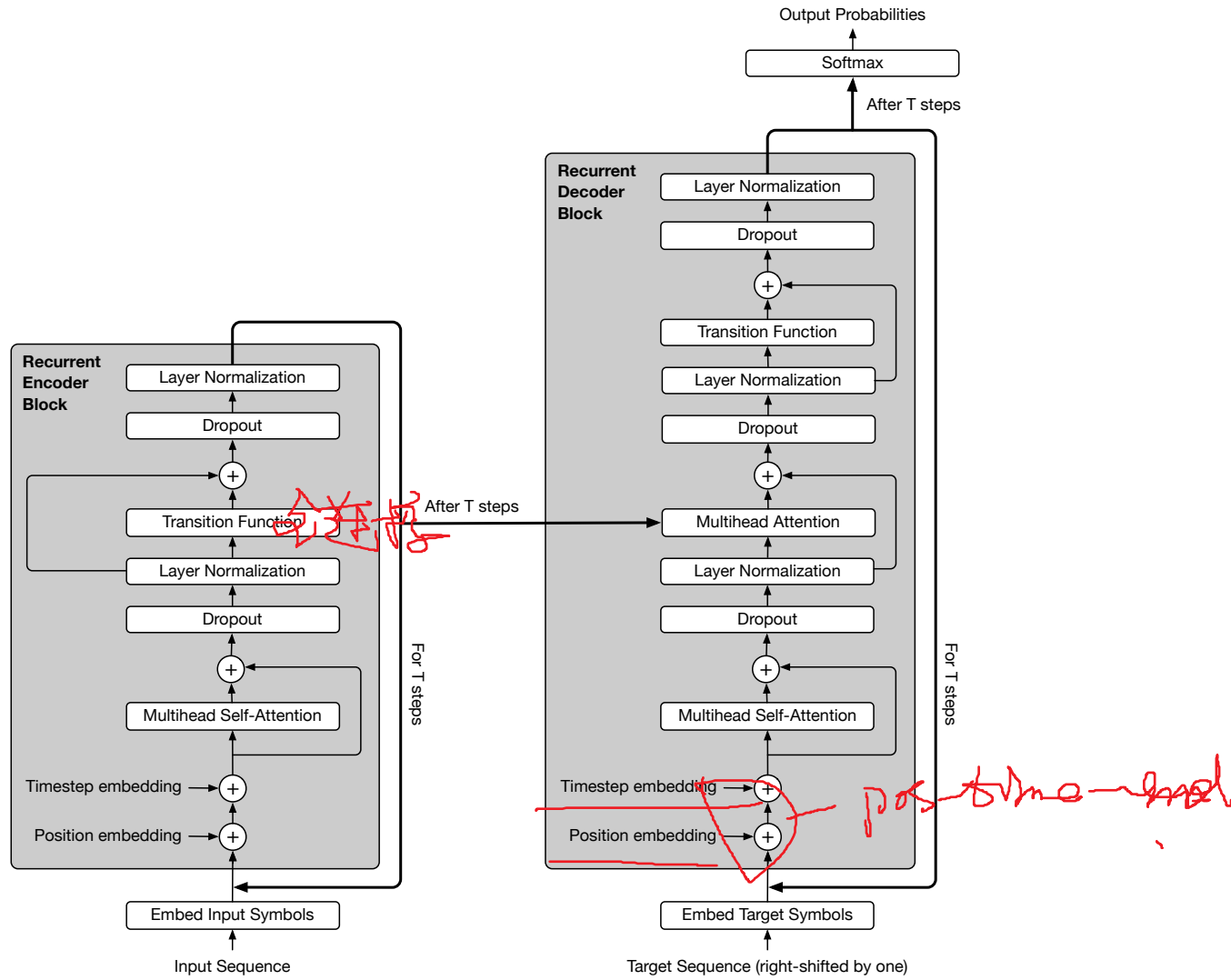


Figure 4: The Universal Transformer with position and step embeddings as well as dropout and layer normalization.

Appendix B bAbI Detailed Results

Best seed run for each task (out of 10 runs)				
Task id	10K		1K	
	train single	train joint	train single	train joint
1	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.5
3	0.4	1.2	3.7	5.4
4	0.0	0.0	0.0	0.0
5	0.0	0.0	0.0	0.5
6	0.0	0.0	0.0	0.5
7	0.0	0.0	0.0	3.2
8	0.0	0.0	0.0	1.6
9	0.0	0.0	0.0	0.2
10	0.0	0.0	0.0	0.4
11	0.0	0.0	0.0	0.1
12	0.0	0.0	0.0	0.0
13	0.0	0.0	0.0	0.6
14	0.0	0.0	0.0	3.8
15	0.0	0.0	0.0	5.9
16	0.4	1.2	5.8	15.4
17	0.6	0.2	32.1	43.2
18	0.0	0.0	0.0	4.1
19	2.8	3.1	47.2	69.11
20	0.0	0.0	2.4	2.4
avg err	0.21	0.29	4.56	7.85
failed	0	0	3	5

Average (\pm var) over all seeds (for 10 runs)				
Task id	10K		1K	
	train single	train joint	train single	train joint
1	0.0 \pm 0.0	0.0 \pm 0.0	0.2 \pm 0.3	0.1 \pm 0.2
2	0.2 \pm 0.4	1.7 \pm 2.6	3.2 \pm 4.1	4.3 \pm 11.6
3	1.8 \pm 1.8	4.6 \pm 7.3	9.1 \pm 12.7	14.3 \pm 18.1
4	0.1 \pm 0.1	0.2 \pm 0.1	0.3 \pm 0.3	0.4 \pm 0.6
5	0.2 \pm 0.3	0.8 \pm 0.5	1.1 \pm 1.3	4.3 \pm 5.6
6	0.1 \pm 0.2	0.1 \pm 0.2	1.2 \pm 2.1	0.8 \pm 0.4
7	0.3 \pm 0.5	1.1 \pm 1.5	0.0 \pm 0.0	4.1 \pm 2.9
8	0.3 \pm 0.2	0.5 \pm 1.1	0.1 \pm 0.2	3.9 \pm 4.2
9	0.0 \pm 0.0	0.0 \pm 0.0	0.1 \pm 0.1	0.3 \pm 0.3
10	0.1 \pm 0.2	0.5 \pm 0.4	0.7 \pm 0.8	1.3 \pm 1.6
11	0.0 \pm 0.0	0.1 \pm 0.1	0.4 \pm 0.8	0.3 \pm 0.9
12	0.2 \pm 0.1	0.4 \pm 0.4	0.6 \pm 0.9	0.3 \pm 0.4
13	0.2 \pm 0.5	0.3 \pm 0.4	0.8 \pm 0.9	1.1 \pm 0.9
14	1.8 \pm 2.6	1.3 \pm 1.6	0.1 \pm 0.2	4.7 \pm 5.2
15	2.1 \pm 3.4	1.6 \pm 2.8	0.3 \pm 0.5	10.3 \pm 8.6
16	1.9 \pm 2.2	0.9 \pm 1.3	9.1 \pm 8.1	34.1 \pm 22.8
17	1.6 \pm 0.8	1.4 \pm 3.4	44.7 \pm 16.6	51.1 \pm 12.3
18	0.3 \pm 0.4	0.7 \pm 1.4	2.3 \pm 3.6	12.8 \pm 9.0
19	3.4 \pm 4.0	6.1 \pm 7.3	50.2 \pm 8.4	73.1 \pm 23.9
20	0.0 \pm 0.0	0.0 \pm 0.0	3.2 \pm 2.5	2.6 \pm 2.8
avg	0.73 \pm 0.89	1.12 \pm 1.62	6.39 \pm 3.22	11.21 \pm 6.62

Appendix C bAbI Attention Visualization

We present visualization of the attention distributions on bAbI tasks for a couple of examples. The visualization of attention weights is over different time steps based on different heads over all the facts in the story and a question. Different color bars on the left side indicate attention weights based on different heads (4 heads in total).

An example from tasks 1: (requiring one supportive fact to solve)

Story:

John travelled to the hallway.
Mary journeyed to the bathroom.
Daniel went back to the bathroom.
John moved to the bedroom

Query:

Where is Mary?

Model's output:

bathroom

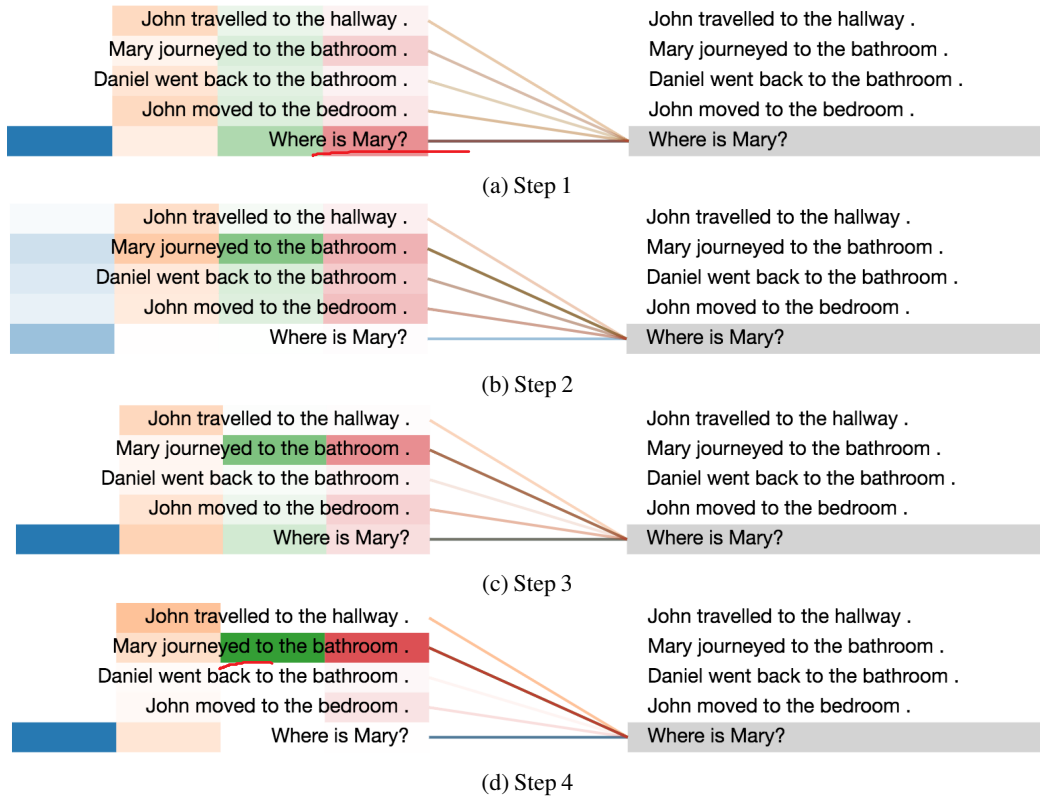


Figure 5: Visualization of the attention distributions, when encoding the question: “Where is Mary?”.

An example from tasks 2: (requiring two supportive facts to solve)

Story:

Sandra journeyed to the hallway.
Mary went to the bathroom.
Mary took the apple there.
Mary dropped the apple.

Query:

Where is the apple?

Model's output:

bathroom

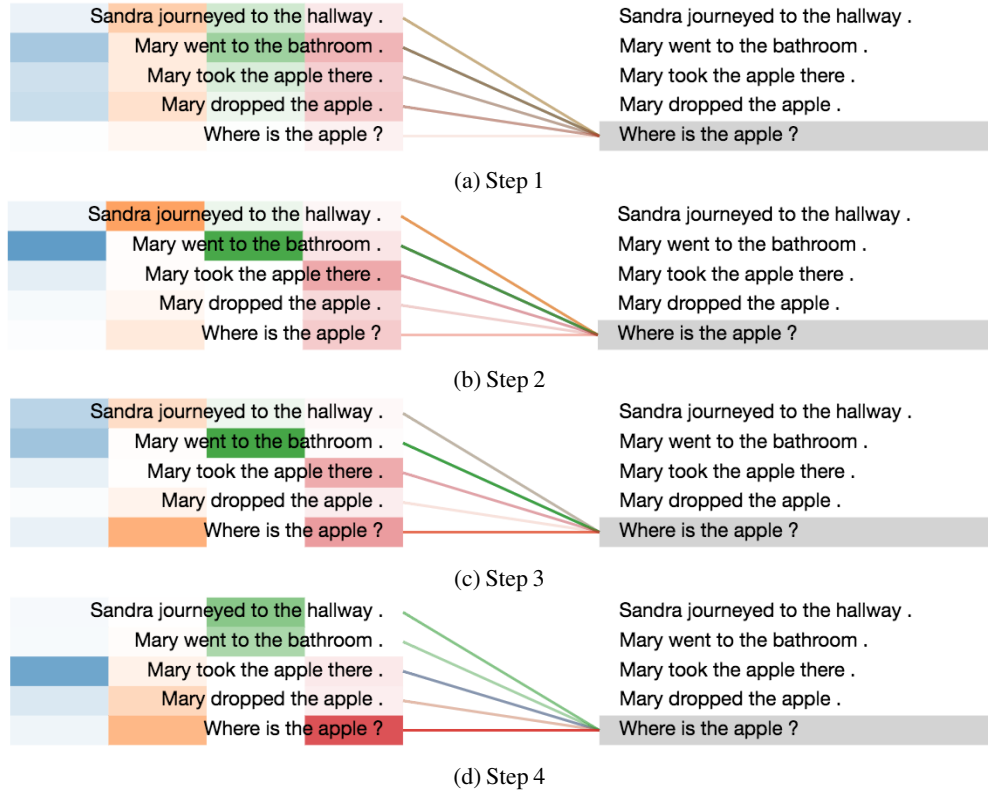


Figure 6: Visualization of the attention distributions, when encoding the question: “Where is the apple?”.

An example from tasks 2: (requiring two supportive facts to solve)

Story:

John went to the hallway.
 John went back to the bathroom.
 John grabbed the milk there.
 Sandra went back to the office.
 Sandra journeyed to the kitchen.
 Sandra got the apple there.
 Sandra dropped the apple there.
 John dropped the milk.

Query:

Where is the milk?

Model's output:

bathroom

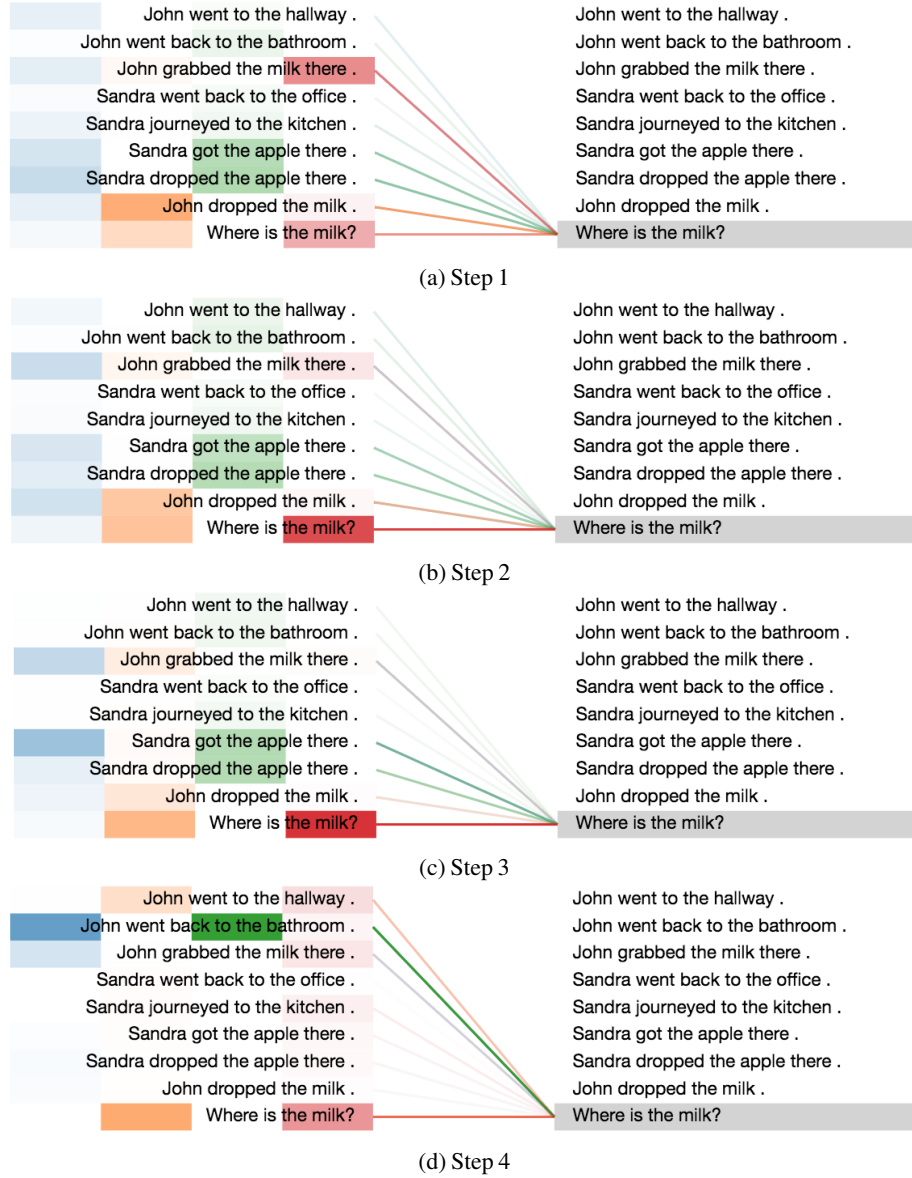


Figure 7: Visualization of the attention distributions, when encoding the question: “Where is the milk?”.

An example from tasks 3: (requiring three supportive facts to solve)

Story:

Mary got the milk.

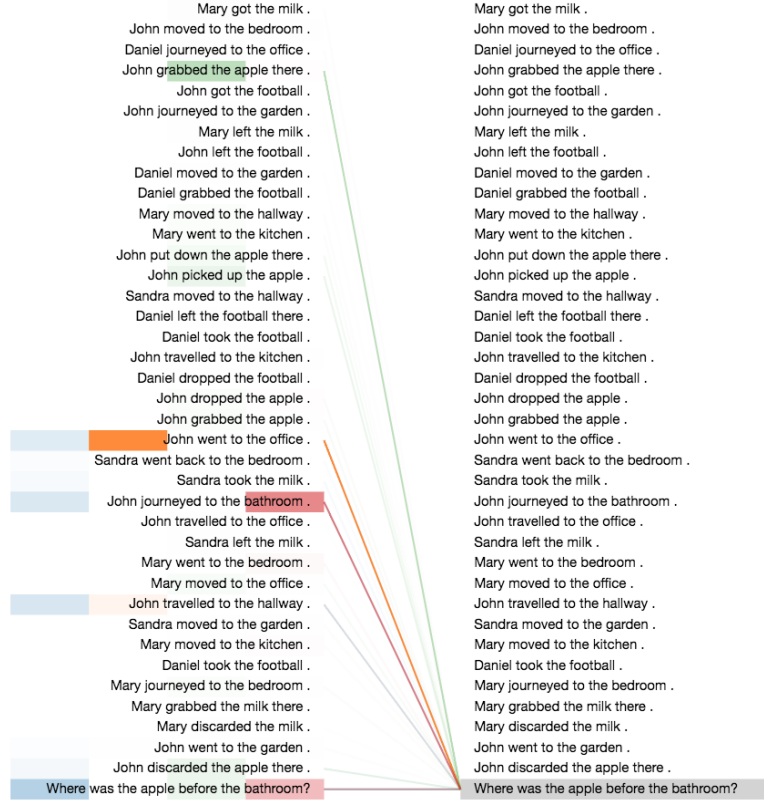
John moved to the bedroom.
Daniel journeyed to the office.
John grabbed the apple there.
John got the football.
John journeyed to the garden.
Mary left the milk.
John left the football.
Daniel moved to the garden.
Daniel grabbed the football.
Mary moved to the hallway.
Mary went to the kitchen.
John put down the apple there.
John picked up the apple.
Sandra moved to the hallway.
Daniel left the football there.
Daniel took the football.
John travelled to the kitchen.
Daniel dropped the football.
John dropped the apple.
John grabbed the apple.
John went to the office.
Sandra went back to the bedroom.
Sandra took the milk.
John journeyed to the bathroom.
John travelled to the office.
Sandra left the milk.
Mary went to the bedroom.
Mary moved to the office.
John travelled to the hallway.
Sandra moved to the garden.
Mary moved to the kitchen.
Daniel took the football.
Mary journeyed to the bedroom.
Mary grabbed the milk there.
Mary discarded the milk.
John went to the garden.
John discarded the apple there.

Query:

Where was the apple before the bathroom?

Model's output:

office



(c) Step 3



(d) Step 4

Figure 8: Visualization of the attention distributions, when encoding the question: “Where was the apple before the bathroom?”.