On the Computational Power of Transformers and Its Implications in Sequence Modeling

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Abstract

Transformers are being used extensively across several sequence modeling tasks. Significant research effort has been devoted to experimentally probe the inner workings of Transformers. However, our conceptual and theoretical understanding of their power and inherent limitations is still nascent. In particular, the roles of various components in Transformers such as positional encodings, attention heads, residual connections, and feedforward networks, are not clear. In this paper, we take a step towards answering these questions. We analyze the computational power as captured by Turing-completeness. We first provide an alternate proof to show that vanilla Transformers are Turing-complete and then we prove that Transformers with positional masking and without any positional encoding are also Turing-complete. We further analyze the necessity of each component for the Turing-completeness of the network; interestingly, we find that a particular type of residual connection is necessary. We demonstrate the practical implications of our results via experiments on machine translation and synthetic tasks.

1 Introduction

Transformer [31] is a recent self-attention based sequence-to-sequence architecture which has led to state of the art results across various NLP tasks including machine translation [17, 31], language modeling [19], question answering [5, 13] and semantic role labeling [27]. Although a number of variants of Transformers have been proposed for different tasks, the original architecture still underlies these variants.

While the training and generalization of machine learning models such as Transformers are the central goals in their analysis, an essential prerequisite to this end is characterization of the computational power of the model: training a model for a certain task cannot succeed if the model is computationally incapable of carrying out the task. While the computational capabilities of recurrent networks (RNNs) have been studied for decades [11, 24], for Transformers we are still in early stages. The celebrated work of [25] showed, assuming arbitrary precision, that RNNs are Turing-complete, meaning that they are capable of carrying out any algorithmic task formalized by Turing machines. Recently, [18] have shown that vanilla Transformers with hard-attention can also simulate Turing machines given arbitrary precision.

The role of various components in the efficacy of Transformers is an important question for further improvements. Recently, some researchers have sought to empirically analyze different aspects of Transformers. [32], [16] investigate the effect of pruning attention heads and their results suggest that different types of attention heads may have different roles in the functioning of the network. Since the Transformer doesn’t process the input sequentially, it requires some form of positional information. Various positional encoding schemes have been proposed to capture order information [22, 3, 9]. At the same time, on machine translation, [34] showed that the performance of Transformers with only positional masking is comparable to that with positional encodings. [30] raised the question of whether explicit
Figure 1: (a) Self Attention with positional encoding, (b) Self Attention with positional masking without positional encoding

encoding is necessary if positional masking is used. Since [18]'s Turing-completeness proof relied heavily on residual connections, they asked whether these connections are essential for Turing-completeness. In this paper, we take a step towards answering such questions.

Our primary goal is to better understand the role of different components with respect to the computational power of the network. The main contributions of our paper are:

(i) We provide an alternate proof to show that Transformers are Turing-complete by directly relating Transformers to RNNs. More importantly, we prove that Transformers with positional masking and without positional encoding are also Turing-complete.

(ii) We analyze the necessity of various components such as self attention blocks, residual connections and feedforward networks for Turing-completeness. Figure 2 provides an overview of our results.

(iii) We explore the implications of our results via experiments on machine translation and synthetic datasets.

2 Related Work

Self Attention Models became popular after the success of Transformers. Several variants were introduced to address the shortcomings of Vanilla Transformers on other seq-to-seq tasks. Variants such as universal Transformers [4] were proposed to improve the performance on learning general algorithms. Efforts were made to combine recurrent and self-attention models [8], [1]. A positional masking based approach to incorporate order information was advocated by [23].

Computational Power of neural networks has been studied since the foundational paper [15]; in particular, this aspect of RNNs has long been studied [11]. The seminal work by [25] showed that RNNs can simulate a Turing machine by using unbounded precision. [2] showed that RNNs with ReLU activations are also Turing-complete. Many recent works have explored the computational power of RNNs in practical settings. The ability of RNNs to recognize counter like languages has been studied by several works [6], [28]. Recently, [33] and [29] showed that LSTMs can learn to exhibit counting like behavior in practice. The ability of RNNs to recognize well bracketed strings has also been recently studied [21], [26]. However, such analysis on Transformers have been relatively scarce.

Theoretical work on Transformers was initiated by [18] who formalized the notion of Transformers and showed that it can simulate a Turing machine given arbitrary precision. [7] showed some limitations of Transformer encoders in modeling regular and context-free languages; however, these are not applicable to the complete Transformer architecture. It has been recently shown that Transformers are universal approximators of sequence to sequence functions given arbitrary precision [35]. With a goal similar to ours, [30] attempted to study the attention mechanism via a kernel formulation. However, a systematic study of various components of Transformer hadn’t been done.
3 Definitions

All the numbers used in our computations will be rational denoted \( \mathbb{Q} \). For a sequence \( \mathbf{X} = (x_1, \ldots, x_n) \), we set \( \mathbf{X}_j := (x_1, \ldots, x_j) \) for \( 1 \leq j \leq n \). We will work with an alphabet \( \Sigma \) of size \( m \), with special symbols \# and \$ signifying the beginning and end of the input sequence, resp. The symbols are mapped to vectors via a given ‘base’ embedding \( f_b : \Sigma \rightarrow \mathbb{Q}^{d_b} \), where \( d_b \) is the dimension of the embedding. E.g., this embedding could be the one used for processing the symbols by the RNN. We set \( f_b(\#) = 0_{d_b} \) and \( f_b(\$) = 0_{d_b} \). Positional encoding is a function \( \text{pos} : \mathbb{N} \rightarrow \mathbb{Q}^{d_b} \). Together, these provide embedding for a symbol \( s \) at position \( i \) given by \( f_b(s) + \text{pos}(i) \), often taken to be simply \( f_b(s) + \text{pos}(i) \).

Vector \( [s] \in \mathbb{Q}^m \) denotes one-hot encoding of \( s \in \Sigma \).

3.1 RNNs

We follow [25] in our definition of RNNs. To feed the sequences \( s_1s_2\ldots s_n \in \Sigma^* \) to the RNN, these are converted to the vectors \( x_1, x_2, \ldots, x_n \) where \( x_i = f_b(s_i) \). The RNN is given by the following recurrence for \( t \geq 1 \)

\[
\mathbf{h}_t = g(W_x\mathbf{x}_{t-1} + W_h\mathbf{h}_{t-1} + \mathbf{b}),
\]

where \( g(\cdot) \) is a multilayer feedforward network (FFN) with activation \( \sigma \), bias vector \( \mathbf{b} \in \mathbb{Q}^{d_b} \), matrices \( W_h \in \mathbb{Q}^{d_b \times d_b} \) and \( W_x \in \mathbb{Q}^{d_b \times d_h} \), and the hidden state \( \mathbf{h}_t \in \mathbb{Q}^{d_b} \) with given initial hidden state \( \mathbf{h}_0 \). \( d_h \) is the hidden state dimension. In their construction, \( g(\cdot) \) is a 4-layer FFN. Note that it is not equivalent to 4-layer stacked RNNs.

After the last symbol \( s_n \) has been fed, we continue to feed the RNN with the terminal symbol \( f_b(\$) \) until it halts. This allows the RNN to carry out computation after having read the input.

**Theorem 3.1.** [25] Any seq-to-seq function \( \Sigma^* \rightarrow \Sigma^* \) computable by a Turing machine can also be computed by an RNN.

For details please see section B.1 in appendix.

3.2 Transformer Architecture

**Vanilla Transformer.** We describe the original Transformer architecture with positional encoding [31] as formalized by [18], with some modifications. All vectors in this subsection are from \( \mathbb{Q}^d \).

The transformer, denoted Trans, is a seq-to-seq architecture. Its input consists of (i) a sequence \( \mathbf{X} = (x_1, \ldots, x_n) \) of vectors, (ii) a seed vector \( \mathbf{y}_0 \). The output is a sequence \( \mathbf{Y} = (y_1, \ldots, y_n) \) of vectors. The sequence \( \mathbf{X} \) is obtained from the sequence \( (s_1, \ldots, s_n) \in \Sigma^{n+1} \) of symbols by using the embedding mentioned earlier: \( x_i = f_b(s_i) + \text{pos}(i) \). The transformer consists of composition of transformer encoder and a transformer decoder. For the feedforward networks in the transformer layers we use the activation as in [25], namely the saturated linear activation function \( \sigma(x) \) which takes value 0 for \( x < 0 \), value \( x \) for \( 0 < x < 1 \) and value 1 for \( x > 1 \). This activation can be easily replaced by the standard ReLU activation via \( \sigma(x) = \text{ReLU}(x) - \text{ReLU}(x-1) \).

**Self-attention.** The self-attention mechanism takes as input (i) a query vector \( \mathbf{q} \), (ii) a sequence of key vectors \( \mathbf{K} = (k_1, \ldots, k_n) \), and (iii) a sequence of value vectors \( \mathbf{V} = (v_1, \ldots, v_n) \). The q-attention over \( \mathbf{K} \) and \( \mathbf{V} \), denoted \( \text{Att}(\mathbf{q}, \mathbf{K}, \mathbf{V}) \), is a vector \( \mathbf{a} = \alpha_1v_1 + \alpha_2v_2 + \cdots + \alpha_nv_n \), where (i) \( \alpha_1, \ldots, \alpha_n \) = \( \rho(f^{\text{att}}(\mathbf{q}, k_1), \ldots, f^{\text{att}}(\mathbf{q}, k_n)) \).

(iii) For vanilla transformers, the scoring function \( f^{\text{att}} \) used is a combination of multiplicative attention [31] and a non-linear function: \( f^{\text{att}}(\mathbf{q}, k_i) = \exp(-|\langle \mathbf{q}, k_i \rangle|) \). This was also used by [18].

**Transformer encoder.** A single-layer encoder is a function \( \text{Enc}(\mathbf{X}; \theta) \), with input \( \mathbf{X} = (x_1, \ldots, x_n) \).
a sequence of vectors in $\mathbb{Q}^d$, and parameters $\theta$. The output is another sequence $Z = (z_1, \ldots, z_n)$ of vectors in $\mathbb{Q}^d$. The parameters $\theta$ specify functions $Q(\cdot), K(\cdot), V(\cdot)$, and $O(\cdot)$, all of type $\mathbb{Q}^d \to \mathbb{Q}^d$. The functions $Q(\cdot), K(\cdot),$ and $V(\cdot)$ are linear transformations and $O(\cdot)$ an FFN. The output $Z$ is computed by $(1 \leq i \leq n)$:

$$a_i = \text{Att}(Q(x_i), K(X), V(X)) + x_i,$$
$$z_i = O(a_i) + a_i.$$ 

The addition operations $+x_i$ and $+a_i$ are the residual connections. The operation in (5) is called the encoder-encoder attention block.

The complete $L$-layer transformer encoder $\text{TEnc}^{(L)}(X; \theta) = (K^e, V^e)$ has the same input $X = (x_1, \ldots, x_n)$ as the single-layer encoder. By contrast, its output $K^e = (k^e_1, \ldots, k^e_\ell)$ and $V^e = (v^e_1, \ldots, v^e_\ell)$ contains two sequences. $\text{TEnc}^{(L)}$ is obtained by composition of $L$ single-layer encoders: let $X^0 := X$, and for $0 \leq \ell \leq L-1$, let $X^{\ell+1} = \text{Enc}(X^\ell; \theta_\ell)$ and finally, $K^e = K^{(\ell)}(X^L)$, $V^e = V^{(\ell)}(X^L)$.

**Transformer decoder.** The input to a single-layer decoder is (i) $(K^e, V^e)$ output by the encoder, and (ii) sequence $Y = (y_1, \ldots, y_k)$ of vectors for $k \geq 1$. The output is another sequence $Z = (z_1, \ldots, z_k)$.

Similar to the single-layer encoder, a single-layer decoder is parameterized by functions $Q(\cdot), K(\cdot), V(\cdot)$ and $O(\cdot)$ and is defined by

$$p_t = \text{Att}(Q(y_t), K(Y_t), V(Y_t)) + y_t,$$
$$a_t = \text{Att}(p_t, K^e, V^e) + p_t,$$
$$z_t = O(a_t) + a_t.$$ 

The operation in (6) will be referred to as the decoder-decoder attention block and the operation in (7) as the decoder-encoder attention block. In (6), positional masking is applied to prevent the network from attending over symbols which are ahead of them.

An $L$-layer Transformer decoder $\text{TDec}^{(L)}((K^e, V^e), Y; \theta) = z$ is obtained by repeated application of $L$ single-layer decoders each with its own parameters and a transformation function $F : \mathbb{Q}^d \to \mathbb{Q}^d$ applied to the last vector in the sequence of vectors output by the final decoder. Formally, for $0 \leq \ell \leq L–1$ and $Y^0 := Y$ we have $Y^{\ell+1} = \text{Dec}((K^e, V^e), Y^\ell; \theta_\ell)$. $z = F(y_L^r)$. Note that while the output of a single-layer decoder is a sequence of vectors, the output of an $L$-layer Transformer decoder is a single vector.

**The complete Transformer.** The output $\text{Trans}(X, y_0) = Y$ is computed by the recurrence $\tilde{y}_{t+1} = \text{TDec}(\text{TEnc}(X), (y_0, y_1, \ldots, y_t))$, for $0 \leq t \leq r – 1$. We get $y_{t+1}$ by adding positional encoding: $y_{t+1} = \tilde{y}_{t+1} + \text{pos}(t+1)$.

**Directional Transformer.** For the directional case, standard multiplicative attention is used, that is, $f^{\text{att}}(q, k_i) = \langle q, k_i \rangle$. The general architecture is the same as for the vanilla case; the differences due to positional masking are the following.

There are no positional encodings. So the input vector $x_i$ only involve $f_b(s_i)$. Similarly, $y_t = \tilde{y}_t$. In (5), $\text{Att}(\cdot)$ is replaced by $\text{Att}(Q(x_i), K(X_i), V(X_i))$ and in (7), $\text{Att}(\cdot)$ is replaced by $\text{Att}(p_t, K^e, V^e)$.

**Remark.** Our definitions deviate slightly from practice, hard-attention being the main one. [7] discusses its practical relevance.

## 4 Primary Results

### 4.1 Turing-Completeness Results

**Theorem 4.1.** The class of Transformer networks with positional encodings is Turing-complete.

**Proof Sketch.** In light of Theorem B.1, it suffices to show that the Transformer can simulate RNNs. The input $s_0, \ldots, s_n \in \Sigma^*$ is provided to the transformer as the sequence of vectors $x_0, \ldots, x_n$, where
We confine our discussion to the case
The class of Transformer networks with positional masking and no explicit positional
Theorem 4.2.
The input
The Transformer takes its input all at once, appending by $v^t$ to $x$; the attention mechanism will recover $x$ at time $t$ and feed it to $O^{\text{dec}}(\cdot)$, thereby simulating the RNN.

As stated earlier, we append the input $s_1, \ldots, s_n$ of the RNN with $\$’s until it halts. Since the Transformer takes its input all at once, appending by $\$’s is not possible (in particular, we do not know how long the computation would take). Instead, we append the input with a single $\$. After encountering a $\$ once, the Transformer will feed (encoding of) $\$ to $O^{\text{dec}}(\cdot)$ in subsequent steps until termination. Here we confine our discussion to the case $t \leq n$; the $t > n$ case is slightly different but simpler.

The construction is simple: it has only one head, one encoder layer and one decoder layer; moreover, the attention mechanisms in the encoder and the decoder-decoder attention layer of the decoder are trivial described below.

The encoder attention layer does trivial computation in that it merely computes the identity function: $z_t = x_t$, which can be easily achieved, e.g. by using the residual connection and setting the value vectors to 0 by setting the function $V^{(0)}(\cdot)$ to identically 0. The final $K^{(1)}(\cdot)$ and $V^{(1)}(\cdot)$ functions bring $(K^e, V^e)$ into useful forms by appropriate linear transformations: $k_t = [0_{d_h}, 0_{d_h}, 0_{d_h}, -1, i]$ and $v_t = [0_{d_h}, f_b(s_i), 0_{d_h}, 0, 0]$. Thus, the key vectors only encode the positional information and the value vectors only encode the input symbols.

The output sequence of the decoder is $y_1, y_2, \ldots$. Our construction will ensure, by induction on $t$, that $y_t$ contains the hidden states $h_t$ of the RNN as a sub-vector along with positional information: $y_t = [h_t, 0_{d_h}, 0_{d_h}, t + 1, 1]$. This is easy to arrange for $t = 0$, and assuming it for $t$ we prove it for $t + 1$.

As for the encoder, the decoder-decoder attention layer acts as the identity: $p_t = y_t$. Now, using the last but one coordinate in $y_t$ representing the time $t + 1$, the attention mechanism $\text{Att}(p_t, K^e, V^e)$ can pick out the embedding of the $t$-th input symbol $x_t$. This is possible because in the key vector $k_t$ mentioned above, almost all coordinates other than the one representing the position $i$ are set to 0, allowing the mechanism to only focus on the positional information and not be distracted by the other contents of $p_t = y_t$: the scoring function has value $f^{\text{att}}(p_t, k_t) = -|\{p_t, k_i\}| = -|i - (t + 1)|$. For a given $t$, it is maximized at $i = t + 1$ for $t < n$ and at $i = n$ for $t \geq n$. This use of scoring function is similar to [18].

At this point, $O^{\text{dec}}(\cdot)$ has at its disposal the hidden state $h_t$ (coming from $y_t$ via $p_t$ and the residual connection) and the input symbol $x_t$ (coming via the attention mechanism and the residual connection). Hence $O(\cdot)$ can act just like the FFN (refer to Lemma D.3) underlying the RNN to compute $h_{t+1}$ and thus $y_{t+1}$, proving the induction hypothesis. The complete construction can be found in Sec. D in the appendix.

\textbf{Theorem 4.2.} The class of Transformer networks with positional masking and no explicit positional encodings is Turing complete.

\textbf{Proof Sketch.} As before, by Theorem B.1 it suffices to show that Transformers can simulate RNNs. The input $s_1, \ldots, s_n$ is provided to the transformer as the sequence of vectors $x_0, \ldots, x_n$, where $x_i = [0_{d_h}, 0_{d_h}, f_b(s_i), [s_i], 0, 0, 0, 0, 0]$. The general idea for the directional case is similar to the vanilla case, namely we would like the FFN $O^{\text{dec}}(\cdot)$ of the decoder to directly simulate the RNN. In the vanilla case, positional encoding and the attention mechanism helped us feed input $x_t$ at the $t$-th iteration of the decoder to $O^{\text{dec}}(\cdot)$. We will implement this scheme but now work with positional masking. We no longer have explicit positional information in the input $x_t$ such as a coordinate with value $t$. The key insight is that in fact we do not need the positional information as such to recover $x_t$ at step $t$: in our construction, the attention mechanism will recover $x_t$ in an indirect manner even though it’s not able to “zero-in” on the $t$-th position.
Let us first explain this without details of the construction. We maintain in vector \( \omega_t \in \mathbb{Q}^{[2]} \), with a coordinate each for symbols in \( \Sigma \), the fraction of times the symbol has occurred up to step \( t \). Now, at a step \( t \leq n \), for the difference \( \omega_t - \omega_{t-1} \) (which is part of the query vector), it can be shown easily that only the coordinate corresponding to \( s_t \) is positive. Thus after applying the linearized sigmoid \( \sigma(\omega_t - \omega_{t-1}) \), we can isolate the coordinate corresponding to \( s_t \). Now using this query vector, the (hard) attention mechanism will be able to pick out the value vectors for all indices \( j \) such that \( s_j = s_t \) and output their average. Crucially, the value vector for an index \( j \) is essentially \( x_j \) which depends only on \( s_j \). Thus, all these vectors are equal to \( x_t \), and so is their average. This recovers \( x_t \), which can now be fed to \( O^{\text{dec}}(\cdot) \), simulating the RNN.

We now outline the construction and relate it to the above discussion. As before, for simplicity we restrict to the case \( t \leq n \). We use only one head, one single-layer encoder and two single-layer decoders. The encoder, as in the vanilla case, does very little other than pass information along. The vectors in \( (K^e, V^e) \) are obtained by the trivial attention mechanism followed by simple linear transformations:

\[
\begin{align*}
K^e_t &= [0_{d_h}, 0_{d_h}, 0_{d_h}, [s_t], 0, 0_m, 0_m, 0_m] \\
V^e_t &= [0_{d_h}, 0_{d_h}, f_0(s_t), 0_m, 0, 0_m, [s_t], 0_m].
\end{align*}
\]

Our construction ensures that at step \( t \) we have \( y_t = [h_{t-1}, 0_{d_h}, 0_{d_h}, 0_m, \frac{1}{2}, 0_m, 0_m, 0_m, \omega_{t-1}] \). As before, the proof is by induction on \( t \).

The first one-layer decoder, the decoder-decoder attention block is trivial: \( p_t^{(1)} = y_t \). In the decoder-encoder attention block, we give equal attention to all the \( t + 1 \) values, which along with \( O^{\text{enc}}(\cdot) \), leads to \( z_t^{(1)} = [h_{t-1}, 0_{d_h}, 0_{d_h}, \delta_t, \frac{1}{2+\tau}, 0_m, 0_m, \omega_t] \), where essentially \( \delta_t = \sigma(\omega_t - \omega_{t-1}) \), except with a change for the last coordinate due to the special status of the last symbol \$ \$ in the processing of RNN.

In the second layer, the decoder-decoder attention block is again trivial with \( p_t^{(2)} = z_t^{(1)} \). We remark that in this construction the scoring function is the standard multiplicative attention. Now \( \langle p_t^{(2)}, k_j \rangle = \langle \delta_t, [s_j] \rangle = \delta_{t,j} \), which is positive if and only if \( s_j = s_t \), as mentioned earlier. Thus attention weights in \( \text{Att}(p_t^{(2)}, K^e_t, V^e_t) \) satisfy \( \text{hardmax}(\langle p_t^{(2)}, k_t^0 \rangle, \ldots, \langle p_t^{(2)}, k_t^f \rangle) = \frac{1}{t} \mathbb{I}(s_0 = s_t), \mathbb{I}(s_1 = s_t), \ldots, \mathbb{I}(s_t = s_t) \), where \( \lambda_t \) is a normalization constant and \( \mathbb{I}(\cdot) \) is the indicator. Refer to Lemma E.3 for more details.

At this point, \( O^{\text{dec}}(\cdot) \) has at its disposal the hidden state \( h_t \) (coming from \( z_t^{(1)} \) via \( p_t^{(2)} \) and the residual connection) and the input symbol \( x_t \) (coming via the attention mechanism and the residual connection). Hence \( O^{\text{dec}}(\cdot) \) can act just like the FFN underlying the RNN to compute \( h_{t+1} \) and thus \( y_{t+1} \).
proving the induction hypothesis. The complete construction can be found in Sec. E in the appendix.

**In practice,** [34] found that for NMT, Transformers with only positional masking achieve comparable performance as compared to the ones with positional encodings. Similar evidence was found by [30]. Our proof for directional transformers entails that there is no loss of order information if positional information is only provided in the form of masking. However, we do not recommend using masking as a replacement for explicit encodings. In practice, one should explore each of the methods and maybe even combinations of encoding and masking. The computational equivalence of encoding and masking given by our results implies that any differences in their performance must come from differences in learning dynamics.

### 4.2 Analysis of Components

The results for various components follow from our construction in Theorem 4.1. Note that in both the encoder and decoder attention blocks, we need to compute the identity function. We can nullify the role of the attention heads by setting the value vectors to zero and making use of only the residual connections to implement the identity function. Thus, even if we remove those attention heads, the model is still Turing complete. On the other hand, we can remove the residual connections around the attention blocks and make use of the attention heads to implement the identity function by using positional encodings. Hence, either the attention head or the residual connection is sufficient to achieve Turing-completeness.

A similar argument can be made for the FFN in the encoder layer: either one of the residual connection or the FFN is sufficient for Turing-completeness. For the decoder-encoder attention head, since it is the only way for the decoder to obtain information about the input, it is necessary for the completeness. The FFN is the only component that can perform computations based on the input and based on the computations performed earlier via recurrence, the model is not Turing complete without it. Figure 2 summarizes the role of different components with respect to the computational expressiveness of the network.

**In practice,** [16] found that removing different kind of attention heads has different degrees of impact on a trained Transformer model. Their results show that removing encoder-decoder attention heads has a more significant impact compared to removing the self attention heads. They suggest that the former heads might be doing most of the heavy lifting. This is in line with our results, namely decoder-encoder attention block is indispensable as opposed to other attention blocks.

**Proposition 4.3.** The class of Transformer networks without residual connection around the decoder-encoder block is not Turing-complete.

**Proof.** The result follows from the observation that without the residual connection, the decoder-encoder attention block gives \( a_t = \text{Att}(p_t, K^e, V^e) \), which leads to \( a_t = \sum_{i=1}^{n} \alpha_i v^e_i \) for some \( \alpha_i \)'s such that \( \sum_{i=1}^{n} \alpha_i = 1 \). Since \( v^e_i \) is produced from the encoder, the vector \( a_t \) will have no information about its previous hidden state values. Since the previous hidden state information was computed and stored in \( p_t \), without the residual connection, the information in \( a_t \) depends solely on the output of the encoder. One could argue that since the attention weights \( \alpha_i \)'s depend on the query vector \( p_t \), one could still glean information from the vectors \( v^e_i \)'s. To see that it’s not always the case, consider any task with a single input and the number of outputs greater than one. Since there is a single input the vector \( a_t \) will be a constant \( (v^e_1) \) at any step and hence the output of the network will always also be constant at all steps. Hence, a model cannot perform such a task. More details can be found in section C.2 in the appendix.

**Discussion.** It’s perhaps surprising that residual connection, originally proposed to assist in the learning of very deep networks, plays a vital role in the computational expressiveness of the network. Without it, the model is limited in its capability to make decisions based on predictions in the previous steps.
5 Experiments

In this section, we explore practical implications of our results. Our experiments are geared towards answering the following questions:

**Q1.** Are there any practical implications of the limitation of Transformers without decoder-encoder residual connections? What kind of tasks can they do, or can not do compared to vanilla Transformers?

**Q2.** Is there any additional benefit of using positional masking as opposed to absolute positional encoding [31]?

Although we showed that Transformers without decoder-encoder residual connection are not Turing complete, it doesn’t imply that they are incapable of performing all the tasks. Our results suggest that it is limited in terms of its capability to make inferences based on its previous computations, which is required for tasks such as counting and language modeling. However, it can be shown that the model is capable of performing tasks which only rely on information provided at a given step such as copying and mapping. For such tasks, given positional information at a particular step, the model can look up the corresponding input and map it via the FFN. We evaluate these hypotheses via our experiments.

| Model                  | Copy Task | Counting |
|------------------------|-----------|----------|
| Vanilla Transformers   | 100.0     | 100.0    |
| - Dec-Enc Residual     | 99.7      | 0.0      |
| - Dec-Dec Residual     | 99.7      | 99.8     |

Table 1: BLEU scores (↑) for copy and counting task. Please see section F for details

For our experiments on synthetic data, we consider two tasks, namely the *copy task* and the *counting task*. For the copy task, the goal of a model is to reproduce the input sequence. We sample sentences of lengths between 5-12 words from Penn Treebank and create the train-test splits with all sentences belonging to the same range of length. In the counting task, we create a very simple dataset where the model is given one number between 0 and 100 as input and its goal is to predict the next five numbers. Since only a single input is provided to the encoder, it is necessary for the decoder to be able to make inferences based on its previous predictions to perform this task. The benefit of conducting these experiments on synthetic data is that they isolate the phenomena we wish to evaluate. We then assess the influence of the limitation on Machine Translation which requires a model to do a combination of both mapping and draw inference from computations in previous timesteps. We evaluate the models on IWSLT’14 German-English dataset and IWSLT’15 English-Vietnamese dataset. For each of these tasks we compare vanilla Transformer with the one without decoder-encoder residual connection. As a baseline we also consider the model without decoder-decoder residual connection, since according to our results, that connection doesn’t influence the computational power of the model. Specifications of the models, experimental setup, datasets and sample outputs can be found in section F in the appendix.

![Figure 3: Performance of the two models on the copy task across varying lengths of test inputs.](image)

**Results** on the effect of residual connections on synthetic tasks can be found in Table 1. As per our hypothesis, all the variants are able to perfectly perform the copy task. For the counting task, the one
| Model                   | De-En | En-Vi |
|------------------------|-------|-------|
| Vanilla Transformers   | 32.9  | 28.8  |
| - Dec-Enc Residual     | 24.1  | 21.8  |
| - Dec-Dec Residual     | 30.6  | 27.2  |

Table 2: BLEU scores (↑) for translation task. Please see section F for details

without decoder-encoder residual connection is theoretically incapable of performing it since the final FFN network at the end of the decoder receives a constant input at every step. However, the other two are able to accomplish it by learning to make decisions based on their prior predictions. For the machine translation task, the results can be found in Table 2. While the drop from removing decoder-encoder residual connection is significant, it’s still able to perform reasonably well since the task can be largely fulfilled by mapping different words from one sentence to another.

For positional masking, our proof technique suggests that due to lack of positional encodings, the model must come up with its own mechanism to make order related decisions. Our hypothesis is that, if it’s able to develop such a mechanism, it should be able to generalize to higher lengths and not overfit on the data it is provided. To evaluate this claim, we simply extend the copy task. We consider two models, one which is provided absolute positional encodings and one where only positional masking is applied. We train both the models for copy tasks on sentences of lengths 5-12 and evaluate it on various lengths going from 5 to 30. Figure 3 shows the performance of these models across various lengths. The model with positional masking clearly generalizes up to higher lengths although its performance too degrades at extreme lengths. We found that the model with absolute positional encodings during training overfits on the fact that the 13th token is always the terminal symbol. Hence, when evaluated on higher lengths it never produces a sentence of length greater than 12. Other encoding schemes such as relative positional encodings [22, 3] can generalize better, since they are inherently designed to address this particular issue. However, our goal is not to propose masking as a replacement of positional encodings, rather it is to determine whether the mechanism that the model develops during training is helpful in generalizing to higher lengths. Note that, positional masking was not devised by keeping generalization or any other benefit in mind. Our claim is only that, the use of masking does not limit the model’s expressiveness and it may benefit in other ways, but during practice one should explore each of the mechanism and even a combination of both. [34] showed that a combination of both masking and encodings is better able to learn order information as compared to explicit encodings.

6 Discussion and Final Remarks

We showed that the class of languages recognized by Transformers and RNNs are exactly the same. This implies that the difference in performance of both the networks across different tasks can be attributed only to their learning capabilities. In contrast to RNNs, Transformers are composed of multiple components which are not essential for its computational expressiveness. However, in practice they may play a crucial role. Recently, [32] showed that the decoder-decoder attention heads in the lower layers of the decoder do play a significant role in the NMT task and suggest that they may be helping in language modeling. This indicates that components which are not essential for the computational power may play a vital role in improving the learning and generalization ability.

Take-Home Messages. We showed that order information can be provided either in the form of explicit encodings or masking without any loss of information. The decoder-encoder attention block plays a necessary role in conditioning the computation on the input sequence while the residual connection around it is necessary to keep track of previous computations. The feedforward network in the decoder is the only component capable of performing computations based on the input and prior computations. Our experimental results show that removing components essential for computational power inhibit the model’s ability to perform certain tasks. At the same time, the components which do not play a role in
the computational power may be vital to the learning ability of the network.

Although our proofs rely on arbitrary precision, which is common practice while studying the computational power of neural networks in theory [25, 18, 7, 35], implementations in practice work over fixed precision settings. However, our construction provides a starting point to analyze Transformer under finite precision. Since RNNs with ReLU activation can recognize all regular languages in finite precision [12], it follows from our construction that Transformer can also recognize a large class of regular languages in finite precision. At the same time, it doesn’t imply that it can recognize all regular languages given the limitation due to the precision required to encode positional information. We leave the study of Transformers in finite precision for future work.

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A Roadmap

We begin with various definitions and results. We define simulation of Turing machines by RNNs and state the Turing-completeness result for RNNs. We define vanilla and directional Transformers and what it means for Transformers to simulate RNNs. Many of the definitions from the main paper are reproduced here, but in more detail. In Sec. C we discuss the effect on computational power of removing various components of Transformers. Sec. D contains the proof of Turing completeness of vanilla Transformers and Sec. E the corresponding proof for directional Transformers. Finally, Sec. F has further details of experiments.

B Definitions

Denote the set \{1, 2, \ldots, n\} by \[n\]. Functions defined for scalars are extended to vectors in the natural way: for a function \(F\) defined on a set \(A\), for a sequence \((a_1, \ldots, a_n)\) of elements in \(A\), we set \(F(a_1, \ldots, a_n) := (F(a_1), \ldots, F(a_n))\). Indicator \(\mathbb{I}(P)\) is 1, if predicate \(P\) is true and is 0 otherwise. For a sequence \(X = (x_{n'}, \ldots, x_n)\) for some \(n' \geq 0\), we set \(X_j := (x_{n'}, \ldots, x_j)\) for \(j \in \{n', i + 1, \ldots, n\}\).

We will work with an alphabet \(\Sigma = \{\#\} \cup \{\beta_1, \ldots, \beta_n\}\), with \(\beta_1 = \#\) and \(\beta_n = \$\). The special symbols \# and \$ correspond to the beginning and end of the input sequence, resp. For a vector \(v\), by \(0_v\) we mean the all-0 vector of the same dimension as \(v\). Let \(t := \min\{t, n\}\).

B.1 RNNs and Turing-completeness

Here we summarize, somewhat informally, the Turing-completeness result for RNNs due to [25]. We recall basic notions from computability theory. In the main paper, for simplicity we stated the results for total recursive functions \(\phi : \{0, 1\}^* \to \{0, 1\}^*\), i.e. a function that is defined on every \(s \in \{0, 1\}^*\) and whose values can be computed by a Turing machine. While total recursive functions form a satisfactory formalization of seq-to-seq tasks, here we state the more general result for partial recursive functions. Let \(\phi : \{0, 1\}^* \to \{0, 1\}^*\) be partial recursive. A partial recursive function is one that need not be defined for every \(s \in \{0, 1\}^*\), and there exists a Turing Machine \(M\) with the following property. The input \(s\) is initially written on the tape of the Turing Machine \(M\) and the output \(\phi(s)\) is the content of the tape upon acceptance which is indicated by halting in a designated accept state. On \(s\) for which \(\phi\) is undefined, \(M\) does not halt.

We now specify how Turing machine \(M\) is simulated by RNN \(R(M)\). In the RNNs in [25] the hidden state \(h_t\) has the form

\[h_t = [q_t, \Psi_1, \Psi_2],\]

where \(q_t = [q_1, \ldots, q_n]\) denotes the state of \(M\) one-hot form. Numbers \(\Psi_1, \Psi_2 \in \mathbb{Q}\), called stacks, store the contents of the tape in a certain Cantor set like encoding (which is similar to, but slightly more involved, than binary representation) at each step. The simulating RNN \(R(M)\), gets as input encodings of \(s_1s_2\ldots s_n\) in the first \(n\) steps, and from then on receives the vector \(0_v\) as input in each step. If \(\phi\) is defined on \(s\), then \(M\) halts and accepts with the output \(\phi(s)\) the content of the tape. In this case, \(R(M)\) enters a special accept state, and \(\Psi_1\) encodes \(\phi(s)\) and \(\Psi_2 = 0\). If \(M\) does not halt then \(R(M)\) also does not enter the accept state.

[25] further show that from \(R(M)\) one can further explicitly produce the \(\phi(s)\) as its output. In the present paper, we will not deal with explicit production of the output but rather work with the definition of simulation in the previous paragraph. This is for simplicity of exposition, and the main ideas are already contained in our results. If the Turing machine computes \(\phi(s)\) in time \(T(s)\), the simulation takes \(O(|s|)\) time to encode the input sequence \(s\) and \(4T(s)\) to compute \(\phi(s)\).

Theorem B.1 ([25]). Given any partial recursive function \(\phi : \{0, 1\}^* \to \{0, 1\}^*\) computed by Turing machine \(M_{\phi}\), there exists a simulating RNN \(R(M_{\phi})\).
In view of the above theorem, for establishing Turing-completeness of Transformers, it suffices to show that RNNs can be simulated by Transformers. Thus, in the sequel we will only talk about simulating RNNs.

B.2 Vanilla Transformer Architecture

Here we describe the original transformer architecture due to [31] as formalized by [18]. While our notation and definitions largely follow [18], they are not identical. The transformer here makes use of positional encoding; later we will discuss the transformer variant using directional attention but without using positional encoding.

The transformer, denoted \( \text{Trans} \), is a sequence-to-sequence architecture. Its input consists of (i) a sequence \( X = (x_1, \ldots, x_n) \) of vectors in \( \mathbb{Q}^d \), (ii) a seed vector \( y_0 \in \mathbb{Q}^d \). The output is a sequence \( Y = (y_1, \ldots, y_r) \) of vectors in \( \mathbb{Q}^d \). The sequence \( X \) is obtained from the sequence \( (s_0, \ldots, s_n) \in \Sigma^{n+1} \) of symbols by using the embedding mentioned earlier: \( x_i = f(b(s_i), \text{pos}(i)) \) for \( 0 \leq i \leq n \). The transformer consists of composition of \( \text{transformer encoder} \) and a \( \text{transformer decoder} \). The transformer encoder is obtained by composing one or more \( \text{single-layer encoders} \) and similarly the transformer decoder is obtained by composing one or more \( \text{single-layer decoders} \). For the feed-forward networks in the transformer layers we use the activation as in [25], namely the saturated linear activation function:

\[
\sigma(x) = \begin{cases} 
0 & \text{if } x < 0, \\
x & \text{if } 0 \leq x \leq 1, \\
1 & \text{if } x > 1.
\end{cases}
\]  

As mentioned in the main paper, we can easily work with the standard ReLU activation via \( \sigma(x) = \text{ReLU}(x) - \text{ReLU}(x-1) \). In the following, after defining these components, we will put them together to specify the full transformer architecture. But we begin with self-attention mechanism which is the central feature of the transformer.

**Self-attention.** The self-attention mechanism takes as input (i) a \( \text{query} \) vector \( q \), (ii) a sequence of \( \text{key} \) vectors \( K = (k_1, \ldots, k_n) \), and (iii) a sequence of \( \text{value} \) vectors \( V = (v_1, \ldots, v_n) \). All vectors are in \( \mathbb{Q}^d \).

The \( q \)-attention over keys \( K \) and values \( V \), denoted by \( \text{Att}(q, K, V) \), is a vector \( a \) given by

\[
(a_1, \ldots, a_n) = \rho(f^{\text{att}}(q, k_1), \ldots, f^{\text{att}}(q, k_n)),
\]

\[
a = \alpha_1 v_1 + \alpha_2 v_2 + \cdots + \alpha_n v_n.
\]

The above definition uses two functions \( \rho \) and \( f^{\text{att}} \) which we now describe. For the normalization function \( \rho : \mathbb{Q}^n \to \mathbb{Q}_{\geq 0}^n \) we will use \( \text{hardmax} \): for \( \mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{Q}^n \), if the maximum value occurs \( r \) times among \( x_1, \ldots, x_n \), then \( \text{hardmax}(\mathbf{x})_i := 1/r \) if \( x_i \) is a maximum value and \( \text{hardmax}(\mathbf{x})_i := 0 \) otherwise. In practice, the softmax is often used but its output values are in general not rational. The names soft-attention and hard-attention are used for the attention mechanism depending on which normalization function is used.

For the Turing-completeness proof of vanilla transformers, the scoring function \( f^{\text{att}} \) used is a combination of multiplicative attention [31] and a non-linear function: \( f^{\text{att}}(q, k_i) = -\langle q, k_i \rangle \). For directional transformers, the standard multiplicative attention is used, that is, \( f^{\text{att}}(q, k_i) = \langle q, k_i \rangle \).

**Transformer encoder.** A \( \text{single-layer encoder} \) is a function \( \text{Enc}(X; \theta) \), where \( \theta \) is the parameter vector and the input \( X = (x_1, \ldots, x_d) \) is a sequence of vector in \( \mathbb{Q}^d \). The output is another sequence \( Z = (z_1, \ldots, z_d) \) of vectors in \( \mathbb{Q}^d \). The parameters \( \theta \) specify functions \( Q(\cdot), K(\cdot), V(\cdot), \) and \( O(\cdot) \), all
of type $Q^d \rightarrow Q^d$. The functions $Q(\cdot), K(\cdot),$ and $V(\cdot)$ are usually linear transformations and this will be the case in our constructions:

$$Q(x_i) = x_i^TW_Q,$$
$$K(x_i) = x_i^TW_K,$$
$$V(x_i) = x_i^TW_V,$$

where $W_Q, W_K, W_V \in Q^{d \times d}$. The function $O(\cdot)$ is a feed-forward network. The single-layer encoder is then defined by

$$a_i = \text{Att}(Q(x_i), K(X), V(X)) + x_i, \quad z_i = O(a_i) + a_i. \quad (5)$$

The addition operations $+x_i$ and $+a_i$ are the residual connections. The operation in (5) is called the encoder-encoder attention block.

The complete $L$-layer transformer encoder $\text{TEnc}^{(L)}(X; \theta)$ has the same input $X = (x_1, \ldots, x_n)$ as the single-layer encoder. By contrast, its output consists of two sequences $(K^e, V^e)$, each a sequence of $n$ vectors in $Q^d$. The encoder $\text{TEnc}^{(L)}(\cdot)$ is obtained by repeated application of single-layer encoders, each with its own parameters; and at the end, two transformation functions $K^e(\cdot)$ and $V^e(\cdot)$ are applied to the sequence of output vectors at the last layer. Functions $K^e(\cdot)$ and $V^e(\cdot)$ are linear transformations in our constructions. Formally, for $1 \leq \ell \leq L - 1$ and $X^\ell := X$, we have

$$X^{\ell+1} = \text{Enc}(X^\ell, \theta),$$
$$K^e = K^{(L)}(X^L),$$
$$V^e = V^{(L)}(X^L).$$

The output of the $L$-layer Transformer encoder $(K^e, V^e) = \text{TEnc}^{(L)}(X)$ is fed to the Transformer decoder which we describe next.

**Transformer decoder.** The input to a single-layer decoder is (i) $(K^e, V^e)$, the sequences of key and value vectors output by the encoder, and (ii) a sequence $Y = (y_1, \ldots, y_k)$ of vectors in $Q^d$. The output is another sequence $Z = (z_1, \ldots, z_k)$ of vectors in $Q^d$.

Similar to the single-layer encoder, a single-layer decoder is parameterized by functions $Q(\cdot), K(\cdot), V(\cdot)$ and $O(\cdot)$ and is defined by

$$p_t = \text{Att}(Q(y_t), K(Y_t), V(Y_t)) + y_t, \quad (6)$$
$$a_t = \text{Att}(p_t, K^e, V^e) + p_t, \quad (7)$$
$$z_t = O(a_t) + a_t.$$

The operation in (6) will be referred to as the *decoder-decoder attention* block and the operation in (7) as the *decoder-encoder attention* block. In the decoder-decoder attention block, positional masking is applied to prevent the network from attending over symbols which are ahead of them.

An $L$-layer Transformer decoder is obtained by repeated application of $L$ single-layer decoders each with its own parameters and a transformation function $F : Q^d \rightarrow Q^d$ applied to the last vector in the sequence of vectors output by the final decoder. Formally, for $1 \leq \ell \leq L - 1$ and $Y^\ell = Y$ we have

$$Y^{\ell+1} = \text{Dec}((K^e, V^e), Y^{\ell}; \theta),$$
$$z = F(y^L_{\ell}).$$

We use $z = \text{TDec}^{L}((K^e, V^e), Y; \theta)$ to denote an $L$-layer Transformer decoder. Note that while the output of a single-layer decoder is a sequence of vectors, the output of an $L$-layer Transformer decoder is a single vector.
The complete Transformer. A Transformer network receives an input sequence \( X \), a seed vector \( y_0 \), and \( r \in \mathbb{N} \). For \( t \geq 0 \) its output is a sequence \( Y = (y_1, \ldots, y_r) \) defined by

\[
\tilde{y}_{t+1} = \text{TD}_{\text{Dec}} \left( \text{TE}_{\text{Enc}}(X), (y_0, y_1, \ldots, y_t) \right).
\]

We get \( y_{t+1} \) by adding positional encoding: \( y_{t+1} = \tilde{y}_{t+1} + \text{pos}(t + 1) \). We denote the complete Transformer by \( \text{Trans}(X; y_0) = Y \). The Transformer “halts” when \( y_T \in H \), where \( H \) is a prespecified halting set.

Simulation of RNNs by Transformers. We say that a Transformer simulates an RNN (as defined in Sec. B.1) if on input \( s \in \Sigma^* \), at each step \( t \), the vector \( y_t \) contains the hidden state \( h_t \) as a subvector: \( y_t = [h_t, \cdot] \), and halts at the same step as RNN.

C Components of Transformers and their effect on computational power

C.1 Encoder

Before moving on to the complete Transformer architecture. We first take a look at the encoder. The Transformer encoder without any positional information is order invariant. That is, given two sequences which are permutations of each other, the output of the network remains the same. Since it is order invariant it cannot recognize regular languages such as \((ab)^*\). \[18\] showed that even though it is permutations invariant it can recognize non-regular languages such as the language \( S = \{ w \in \{a, b\}^* | w \text{ has strictly more symbols } a \text{ than } b \} \). However, it is trivial to see that even though it can compare the occurrence of two symbols, it cannot recognize well-balanced parenthesis languages such as Dyck-1. Let \( \Sigma = \{[ ], \} \), then the language Dyck-1 denoted by \( L_D \) is defined as \( L_D = \{ w \in \Sigma^* | \text{ all prefixes of } w \text{ contain no more } [ \text{ 's than } ] \text{'s and the number of } [ \text{'s in } w \text{ equals the number of } ] \text{'s } \} \). Essentially the number of open brackets have to be greater than the number of closed brackets at every point and the total number of open and closed brackets should be the same at the end.

Proposition C.1. There exists a Transformer Encoder with positional masking that can recognize the language \( L_D \) (Dyck-1)

Proof. Let \( s_1, s_2, \ldots, s_n \) denote a sequence \( w \in L_D \). Let \( f_e([]) = 1 \) and \( f_e(\cdot) = -1 \). We use a single layer Encoder network where we set the weight matrix for key vectors to be null matrix, that is \( W_k = 0 \). The weights matrices corresponding query and value vectors are set to Identity. Thus,

\[
\text{Att}(q_i, K_i, V_i) = \sum_{j=1}^i v_j
\]

for \( 1 \leq i \leq n \). Thus if in the first \( i \) inputs there are \( k \) open brackets and \( l \) closed brackets, then \( a_i = \frac{1}{k} - \frac{1}{l} \) where \( i = k + l \). This implies that if \( a_i \) is greater than zero then, the number of open brackets higher and if its less than zero then the number of closed brackets are higher. We then use a simple feedforward network of the form \( z_i = \text{ReLU}(W_1 a_i) \) where \( W_1 \in \mathbb{Q}^{2} \). Let \( W_1 = [1, -1] \), then \( z_i = \text{ReLU}([a_i, -a_i]) \). The first coordinate of \( z_i \) will be nonzero only when the number of open brackets will be greater than the number of closed brackets and zero otherwise. Similarly, the second coordinate will be nonzero only when the number of closed brackets are greater than the number of open brackets and will be zero otherwise. Thus for the for a word \( w \) to be in language \( L_D \), the second coordinate must never be nonzero and the first coordinate of \( z_n \) should be zero to ensure the number of open brackets and closed brackets are the same.

For an input sequence \( s_1, s_2, \ldots, s_n \), the encoder will produce \( z_1, \ldots, z_n \) based on the construction specified above. A word \( w \) belongs to language \( L_D \) if \( z_{i,2} = 0 \) for all \( 1 \leq i \leq n \) (maxpool over \( z_{i,2} \)) and \( z_{n,1} = 0 \). Else, the word \( w \) does not belong to the language \( L_D \). \(\square\)
The task of recognizing the language Dyck-1 is similar to the task of comparing the occurrences of symbols $a$ and $b$ in $\Sigma^*$ where $\Sigma = a, b$. The main difference being that the order also matters. For an Encoder without any positional information, the sequence $[]$ and $[]$ will lead to the same outputs whereas for an Encoder with positional masking, it will be able to distinguish the two and recognize the one that belongs to Dyck-1.

### C.2 Residual Connections

**Proposition C.2.** The Transformer without residual connection around the Encoder-Decoder Attention block in the Decoder is not Turing Complete

**Proof.** Recall that the vectors $a_t$ is produced from the Encoder-Decoder Attention block in the following way,

$$a_t = \text{Att}(p_t, K^e, V^e) + p_t$$

The result follows from the observation that without the residual connections, $a_t = \sum_{i=1}^n \alpha_i v^e_i$ for some $\alpha_i$s such that $\sum_{i=1}^n \alpha_i = 1$. Since $v^e_i$ is produced from the encoder, the vector $a_t$ will have no information about its previous hidden state values. Since the previous hidden state information was computed and stored in $p_t$, without the residual connection, the information in $a_t$ depends solely on the output of the encoder.

One could argue that since the attention weights $\alpha_i$s depend on the query vector $p_t$, it could still use it gain the necessary information from the vectors $v^e_i$s. To see that its not true, consider the following simple problem, given a value $\Delta$, where $0 \leq \Delta \leq 1$, the network has to produce the values $0, \Delta, 2\Delta, \ldots, 1$. That is, it has to produce values of the form $n\Delta$ for all $n$ such that $n\Delta \in [0, 1]$. Note that, since there is only one input, the encoder will produce only one particular output vector and regardless of what the value of the query vector $p_t$ is, the vector $a_t$ will be constant at every timestep. Since $a_t$ is fed to feedforward network which maps it to $z_t$, the output of the decoder will remain the same at every timestep and it cannot produce distinct values. Thus the model cannot perform the task defined above which RNNs and Vanilla Transformers can easily do with a simple counting mechanism via their recurrent connection.

In case of hard attention, the network without Encoder-Decoder residual connection with $n$ inputs can have atmost $2^n - 1$ distinct $a_t$ values and hence will be unable to perform a task that takes $n$ inputs and has to produce more than $2^n - 1$ outputs.

This implies that the model without Encoder-Decoder residual connection is limited in its capability to perform tasks which requires it to make inferences based on previously generated outputs.

### D Completeness of Vanilla Transformers

#### D.1 Simulation of RNNs by Transformers with positional encoding

**Theorem D.1.** RNNs can be simulated by vanilla Transformers and hence the class of vanilla Transformers is Turing-complete.

**Proof.** The construction of the simulating transformer is simple: it uses a single head and both the encoder and decoder have one layer. Moreover, the encoder does very little and most of the action happens in the decoder. The main task for the simulation is to design the input embedding (building on the given base embedding $f_b$), the feedforward network $O(\cdot)$ and the matrices corresponding to functions $Q(\cdot), K(\cdot), V(\cdot)$.

**Input embedding.** The input embedding is obtained by summing the symbol and positional encodings which we next describe. These encodings have dimension $d = 2d_h + d_b + 2$, where $d_h$ is the dimension of the hidden state of the RNN and $d_b$ is the dimension of the given encoding $f_b$ of the input symbols.
We will use the symbol encoding \( f_{\text{symb}} : \Sigma \rightarrow \mathbb{Q}^d \) which is essentially the same as \( f_b \) except that the dimension is now larger:

\[
  f_{\text{symb}}(s) = [0, f_b(s); 0, 0, 0].
\]

The positional encoding \( \text{pos} : \mathbb{N} \rightarrow \mathbb{Q}^d \) is simply

\[
  \text{pos}(i) = [0, 0, 0, i, 1].
\]

Together, these define the combined embedding \( f \) for a given input sequence \( s_0s_1 \cdots s_n \in \Sigma^* \) by

\[
  f(s_i) = f_{\text{symb}}(s_i) + \text{pos}(i) = [0, f_b(s_i), 0, i, 1].
\]

The vectors \( v \in \mathbb{Q}^d \) used in the computation of our transformer are of the form

\[
  v = [h_1, s, h_2, x_1, x_2],
\]

where \( h_1, h_2 \in \mathbb{Q}^{d_h}, s \in \mathbb{Q}^{d_s}, \) and \( x_1, x_2 \in \mathbb{Q} \). The coordinates corresponding to the \( h_i \)'s are reserved for computation related to hidden states of the RNN, the coordinates corresponding to \( s \) are reserved for base embeddings, and those for \( x_1 \) and \( x_2 \) are reserved for scalar values related to positional operations. The first two blocks, corresponding to \( h_1 \) and \( s \) are reserved for computation of the RNN.

During the computation of the Transformer, the underlying RNN will get the input \( s_t \) at step \( t \) for \( t = 0, 1, \ldots \), where recall that \( \bar{t} = \min\{t, n\} \). This sequence leads to the RNN getting the embedding of the input sequence \( s_0, \ldots, s_n \) in the first \( n + 1 \) steps followed by the embedding of the symbol \( \$ \) for the subsequent steps, which is in accordance with the requirements of \cite{25}. Similar to \cite{18} we use the following scoring function in the attention mechanism in our construction,

\[
  f_{\text{att}}(q_i, k_j) = -|\langle q_i, k_j \rangle| \tag{8}
\]

**Construction of TEnc.** As previously mentioned, our transformer encoder has only one layer, and the computation in the encoder is very simple: the attention mechanism is not utilized, only the residual connections are. This is done by setting the matrix for \( V(\cdot) \) to the all-zeros matrix, and the feedforward networks to always output \( 0 \). The application of appropriately chosen linear transformations for the final \( K(\cdot) \) and \( V(\cdot) \) give the following lemma about the output of the encoder.

**Lemma D.2.** There exists a single layer encoder denoted by \( \text{TEnc} \) that takes as input the sequence \( (x_1, \ldots, x_n, \$) \) and generates the tuple \( (K^e, V^e) \) where \( K^e = (k_1, \ldots, k_n) \) and \( V^e = (v_1, \ldots, v_n) \) such that,

\[
  k_i = [0, 0, 0; h_1, -1, i],
  v_i = [0, s_i; h_1, 0, 0].
\]

**Construction of TDec.** As in the construction of TEnc, our TDec has only one layer. Also like TEnc, the decoder-decoder attention block just computes the identity: we set \( V^{(1)}(\cdot) = 0 \) identically, and use the residual connection so that \( p_t = y_t \).

For \( t \geq 0 \), at the \( t \)-th step we denote the input to the decoder as \( y_t = \tilde{y}_t + \text{pos}(t) \). Let \( h_0 = 0 \) and \( y_0 = 0 \). We will show by induction that at the \( t \)-th timestep we have

\[
  y_t = [h_t, 0, 0; h_1, t + 1, 1]. \tag{9}
\]

By construction, this is true for \( t = 0 \):

\[
  y_0 = [0, 0, 0; h_1, 1, 1].
\]

Assuming that it holds for \( t \), we show it for \( t + 1 \).
By Lemma D.4
\[
\text{Att}(p_t, K^e, V^e) = [0_h, s_{t+1}; 0_h, 0, 0].
\] (10)

Lemma D.4 basically shows how we retrieve the input \(s_{t+1}\) at the relevant step for further computation in the decoder. It follows that
\[
\alpha_t = \text{Att}(p_t, K^e, V^e) + p_t = [h_t, s_{t+1}; 0_h, t+1, 1].
\]

In the final block of the decoder, the computation for RNN takes place:

**Lemma D.3.** There exists a function \(O(\cdot)\) defined by feed-forward network such that,
\[
O(\alpha_t) = [(h_{t+1} - h_t), -s_{t+1}, 0_h, -(t + 1), -1],
\]
where \(W_h, W_v\) and \(b\) denote the parameters of the RNN under consideration.

This leads to
\[
z_t = O(\alpha_t) + \alpha_t = [h_{t+1}, 0_s; 0_h, 0, 0].
\]

We choose the function \(F\) for our decoder to be the identity function, therefore
\[
\tilde{y}_{t+1} = [h_{t+1}, 0_s; 0_h, 0, 0],
\]
which means \(y_{t+1} = \tilde{y}_{t+1} + \text{pos}(t+1) = [h_{t+1}, 0_s; 0_h, t + 2, 1]\), proving our induction hypothesis.

### D.2 Technical Lemmas

**Proof of Lemma D.2.** We construct a single-layer encoder achieving the desired \(K^e\) and \(V^e\). We make use of the residual connections and via trivial self-attention we get that \(z_i = x_i\). More specifically for \(i \in [n]\) we have
\[
V^{(1)}(x_i) = 0,
\]
\[
\alpha_i = 0 + x_i,
\]
\[
O(\alpha_i) = 0,
\]
\[
z_i = 0 + \alpha_i = x_i.
\]

\(V^{(1)}(x_i) = 0\) can be achieved by setting the weight matrix as the all-0 matrix. Recall that \(x_i\) is defined as
\[
x_i = \begin{bmatrix} 0_h, s_i, \\ 0_h, i, 1 \end{bmatrix}.
\]

We then apply linear transformations in \(K(z_i) = z_i W_k\) and \(V(z_i) = z_i W_v\), where
\[
W_k^T = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & -1 & 0 \end{bmatrix},
\]
and \(W_k \in \mathbb{Q}^{d \times d}\), and similarly one can obtain \(v_i\) by setting the submatrix of \(W_v \in \mathbb{Q}^{d \times d}\) formed by the first \(d - 2\) rows and columns to the identity matrix, and the rest of the entries to zeros.

**Lemma D.4.** Let \(q_t \in \mathbb{Q}^d\) be a query vector such that \(q = [\cdot, \ldots, \cdot, t+1, 1]\) where \(t \in \mathbb{N}\) and \(\cdot, \cdot\) denotes an arbitrary value. Then we have
\[
\text{Att}(q_t, K^e, V^e) = [0_h, s_{t+1}; 0_h, 0, 0].
\] (11)
Proof. Recall that \( p_t = y_t = [h_t, 0, \ldots, 0, t + 1, 1] \) and \( k_i = [0, 0, \ldots, 0, -1, i] \) and hence
\[
\langle p_t, k_i \rangle = i - (t + 1),
\]
\[
f^{\text{att}}(p_t, k_i) = -|i - (t + 1)|.
\]
Thus, for \( i \in [n] \), the scoring function \( f^{\text{att}}(p_t, k_i) \) has the maximum value 0 at index \( i = t + 1 \) if \( t < n \); for \( t \geq n \), the maximum value \( t + 1 - n \) is achieved for \( i = n \). Therefore
\[
\text{Att}(p_t, K^e, V^e) = s_{t+1}.
\]

Proof of Lemma D.3. Recall that
\[
a_t = [h_t, s_{t+1}, 0_h, t + 1, 1]
\]
Network \( O(a_t) \) is of the form
\[
O(a_t) = W_2 \sigma(W_1 a_t + b_1),
\]
where \( W_i \in \mathbb{Q}^{d \times d} \) and \( b \in \mathbb{Q}^d \) and
\[
W_1 = \begin{bmatrix}
  d_h & d_e & d_h & 2 \\
  d_h & 0 & \ & 0 \\
  d_h & 1 & 0 & 0 \\
  2 & 0 & 0 & 1
\end{bmatrix}
\]
and \( b_1 = [b_h, 0_s, 0_h, 0, 0] \). Hence
\[
\sigma(W_1 a_t + b_1) = [\sigma(W_h h_t + W_x s_{t+1} + b), s_{t+1}, h_t, t + 1, 1]
\]
Next we define \( W_2 \) by
\[
W_2 = \begin{bmatrix}
  d_h & d_e & d_h & 2 \\
  d_h & 1 & 0 & -1 & 0 \\
  d_h & 0 & -1 & 0 & 0 \\
  2 & 0 & 0 & 0 & -1
\end{bmatrix}
\]
This leads to
\[
O(a_t) = W_2 \sigma(W_1 a_t + b_1)
\]
\[
= [\sigma(W_h h_t + W_x s_{t+1} + b) - h_t, -s_{t+1}, h_t, -(t + 1), -1],
\]
which is what we wanted to prove. \( \square \)

E Completeness of Directional Transformers

There are a few changes in the architecture of the Transformer to obtain directional Transformer. The first change is that there are no positional encodings and thus the input vector \( x_i \) only consists of \( s_i \). Similarly, there are no positional encodings in the decoder inputs and hence \( y_t = \tilde{y}_t \). The vector \( \tilde{y} \) is the output representation produced at the previous step and the first input vector to the decoder \( \tilde{y}_0 = 0 \). Instead of using positional encodings, we apply positional masking to the inputs and outputs of the encoder.
Thus the encoder-encoder attention in (5) is redefined as
\[ a_i^{(l+1)} = \text{Att}(Q(z_i^{(l)}), K(Z_i^{(l)}), V(Z_i^{(l)})) + z_i^{(l)}, \]
where \( Z^{(0)} = X \). Similarly the decoder-encoder attention in (7) is redefined by
\[ a_t^{(l)} = \text{Att}(p_t^{(l)}, K_t^{e}, V_t^{e}) + p_t^{(l)}, \]
where \( l \) in \( a_t^{(l)} \) denotes the layer \( l \) and we use \( v^{(l,b)} \) to denote any intermediate vector being used in \( l \)-th layer and \( b \)-th block in cases where the same symbol is used in multiple blocks in the same layer.

**Theorem E.1.** RNNs can be simulated by vanilla Transformers and hence the class of vanilla Transformers is Turing-complete.

**Proof.** The Transformer network in this case will be more complex than the construction for the vanilla case. The encoder remains very similar, but the decoder is different and has two layers.

**Embedding.** We will construct our Transformer to simulate an RNN of the form given in the definition with the recurrence
\[ h_t = g(W_h h_{t-1} + W_x x_t + b). \]
The vectors used in the Transformer layers are of dimension \( d = 2d_h + d_e + 4|\Sigma| + 1 \). Where \( d_h \) is the dimension of the hidden state of the RNN and \( d_e \) is the dimension of the input embedding.

All vector \( v \in \mathbb{Q}^d \) used during the computation of the network are of the form
\[ v = [h_1, h_2, s_1, \|s_1\|, x_1, \|s_2\|, \|s_3\|, \|s_4\|] \]
where \( h_i \in \mathbb{Q}^{d_h}, s \in \mathbb{Q}^{d_e} \) and \( x_i \in \mathbb{Q} \). These blocks reserved for different types of objects. The vectors \( h_{i:s} \) are reserved for computation related to hidden states of RNNs, \( s_{i:s} \) are reserved for input embeddings and \( x_{i:s} \) are reserved for scalar values related to positional operations.

Given an input sequence \( s_0 s_1 s_2 \cdots s_n \in \Sigma^* \) where \( s_0 = \# \) and \( s_n = $ \), we use an embedding function \( f : \Sigma \rightarrow \mathbb{Q}^d \) defined as
\[ f(s_i) = x_i = \begin{bmatrix} 0_{i_h}, 0_{i_h}, s_i, \|s_i\|, 0, 0_{i_o}, 0_{i_o}, 0_{i_o} \end{bmatrix} \]

Unlike [18], we use the following scoring function similar to [31] in the attention mechanism in our construction,
\[ f^{\text{att}}(q_i, k_j) = \langle q_i, k_j \rangle. \]

For the computation of the Transformer, we also use a vector sequence in \( \mathbb{Q}^{|\Sigma|} \) defined by
\[ \omega_t = \frac{1}{t+1} \sum_{j=0}^{t} \|s_j\|, \]
where \( 0 \leq t \leq n \). The vector \( \omega_t = (\omega_{t,1}, \ldots, \omega_{t,|\Sigma|}) \) contains the proportion of each input symbol till step \( t \) for \( 0 \leq t \leq n \). Set \( \omega_{-1} = 0 \). From the definition of \( \omega_t \), it follows that at any step \( 1 \leq k \leq |\Sigma| \) we have
\[ \omega_{t,k} = \frac{\phi_{t,k}}{t+1}, \]  
where \( \phi_{t,k} \) denotes the number of times the \( k \)-th symbol \( \beta_k \) in \( \Sigma \) has appeared till the \( t \)-th step. Note that \( \omega_{t,0} = \frac{1}{t+1} \) since the first coordinate corresponds to the proportion of the start symbol \( \# \) which appears only once at \( t = 0 \). Similarly, \( \omega_{t,|\Sigma|} = 0 \) for \( 0 \leq t < n \) and \( \omega_{t,|\Sigma|} = 1/(t+1) \) for \( t \geq n \), since the end symbol \$ doesn’t appear till the end of the input and it appears only once at \( t = n \).
We define two more sequences of vectors in $\mathbb{Q}^{[\Sigma]}$ for $0 \leq t \leq n$:
\[
\Delta_t = \sigma(\omega_t - \omega_{t-1}), \\
\delta_t = (\Delta_{t,1}, \ldots, \Delta_{t,|\Sigma|-1}, 1/2^{t+1}).
\]
Here $\Delta_t$ denotes the difference in the proportion of symbols between the $t$-th and $(t-1)$-th steps, with the application of sigmoid activation. In vector $\delta_t$, the last coordinate of $\Delta_t$ has been replaced with $1/2^{t+1}$. The last coordinate in $\omega_t$ indicates the proportion of the terminal symbol $\mathbb{S}$ and hence the last value in $\Delta_t$ denotes the change in proportion of $\mathbb{S}$. We set the last coordinate in $\delta_t$ to an exponentially decreasing sequence so that after $n$ steps we always have a nonzero score for the terminal symbol and it is taken as input in the underlying RNN. Different and perhaps simpler choices for the last coordinate of $\delta_t$ may be possible. Note that $0 \leq \Delta_{t,k} \leq 1$ and $0 \leq \delta_{t,k} \leq 1$ for $0 \leq t \leq n$ and $1 \leq k \leq |\Sigma|$.

**Construction of TEnc.** The input to the network $\text{DTrans}_M$ is the sequence $(s_0, s_1, \ldots, s_{n-1}, s_n)$ where $s_0 = \#$ and $s_n = \mathbb{S}$. Our encoder is a simple single layer network such that $\text{TEnc}(x_0, x_1, \ldots, x_n) = (K^e, V^e)$ where $K^e = (k^e_0, \ldots, k^e_n)$ and $V^e = (v^e_0, \ldots, v^e_n)$ such that,
\[
k^e_i = \begin{bmatrix} 0_h & 0_h & 0_s \\ [s_i], 0, 0_w, 0_w, 0_w \end{bmatrix}, \\
v^e_i = \begin{bmatrix} 0_h & 0_h & s_i, \\ 0_w, 0_w, [s_i], 0_w \end{bmatrix}.
\]
Similar to our construction of the encoder for vanilla transformer (Lemma D.2), the above $K^e$ and $V^e$ can be obtained by making the output of $\text{Att}(\cdot) = 0$ by choosing the $V(\cdot)$ to always evaluate to 0 and similarly for $O(\cdot)$, and using residual connections. Then one can produce $K^e$ and $V^e$ via simple linear transformations using $K(\cdot)$ and $V(\cdot)$.

**Construction of TDec.** At the $t$-th step we denote the input to the decoder as $y_t = \tilde{y}_t$, where $0 \leq t \leq r$, where $r$ is the step where the decoder halts. Let $h_{-1} = 0_h$ and $h_0 = h_i$. We will prove by induction on $t$ that for $0 \leq t \leq r$ we have
\[
y_t = \begin{bmatrix} h_{t-1}, 0_h, 0_s, \\ 0_w, \frac{1}{t}, 0_w, 0_w, \omega_{t-1} \end{bmatrix}.
\]
(14)
This is true for $t = 0$ by the choice of seed vector:
\[
y_0 = \begin{bmatrix} 0_h, 0_h, 0_s, \\ 0_w, 1, 0_w, 0_w, 0_w \end{bmatrix}.
\]
Assuming the truth of (14) for $t$, we show it for $t + 1$.

**Layer 1.** Similar to the construction in Lemma D.2, in the decoder-decoder attention block we set $V^{(1)}(\cdot) = 0_d$ and use the residual connections to set $p_t^{(1)} = y_t$. At the $t$-th step in the decoder-encoder attention block of layer 1 we have
\[
\text{Att}(p_t^{(1)}, K^e_t, V^e_t) = \sum_{j=0}^t \alpha_{t,j}^{(1,2)} v^e_j,
\]
where
\[
(\alpha_{t,1}^{(2,2)}, \ldots, \alpha_{t,t}^{(2,2)}) = \text{hardmax} \left( (p_t^{(1)}, k^e_t), \ldots, (p_t^{(1)}, k^e_t) \right) = \text{hardmax}(0, \ldots, 0) = \left( \frac{1}{t+1}, \ldots, \frac{1}{t+1} \right).
\]
Therefore
\[ \sum_{j=0}^{t} \alpha_{t,j}^{(1,2)} v_{j}^{e} = \begin{bmatrix} 0_{h}, 0_{h}, s_{0:t}, 0_{\omega}, 0_{\omega}, \omega_{t}, 0_{\omega} \end{bmatrix} \]

where
\[ s_{0:t} = \frac{1}{t+1} \sum_{j=0}^{t} s_{j}. \]

Thus,
\[ \alpha_{t}^{(1)} = \text{Att}(p_{t}^{(1)}, K_{t}^{e}, V_{t}^{e}) + p_{t}^{(1)} = [h_{t-1}, 0_{h}, s_{0:t}, 0_{\omega}, 1_{t}, 0_{\omega}, \omega_{t}, \omega_{t-1}]. \]

In Lemma E.2 we construct feed-forward network \( O^{(1)}(\cdot) \) such that
\[ O^{(1)}(\alpha_{t}^{(1)}) = [0_{h}, 0_{h}, -s_{0:t}, \delta_{t}, -\frac{1}{2t} + \frac{1}{2t+1}, 0_{\omega}, -\omega_{t}, -\omega_{t-1} + \omega_{t}]. \]

Hence
\[ z_{t}^{(1)} = O^{(1)}(\alpha_{t}^{(1)}) + \alpha_{t}^{(1)} = [h_{t-1}, 0_{h}, 0_{s}, \delta_{t}, \frac{1}{2t+1}, 0_{\omega}, 0_{\omega}, 0_{\omega}, 0_{\omega}]. \]

\textbf{Layer 2.} In the first block of layer 2, we set the value transformation function to identically zero similar to Lemma D.2, i.e. \( V^{(2)}(\cdot) = 0 \) which leads to the output of \( \text{Att}(\cdot) \) to be 0 and then using the residual connection we get \( p_{t}^{(2)} = z_{t}^{(1)}. \) It follows by Lemma E.3 that
\[ \text{Att}(p_{t}^{(2)}, K_{t}^{e}, V_{t}^{e}) = [0_{h}, 0_{h}, s_{t}, 0_{\omega}, 0_{\omega}, \|s_{t}\|, 0_{\omega}]. \]

Thus,
\[ \alpha_{t}^{(2)} = \text{Att}(p_{t}^{(2)}, K_{t}^{e}, V_{t}^{e}) + p_{t}^{(2)} = [h_{t-1}, 0_{h}, s_{t}, \delta_{t}, 1_{t}, 0_{\omega}, \|s_{t}\|, \omega_{t}]. \]

In the final block of the decoder in the second layer, the computation for RNN takes place. In Lemma E.4 below we construct the feed-forward network \( O^{(2)}(\cdot) \) such that
\[ O^{(2)}(\alpha_{t}^{(2)}) = [\sigma(W_{h} h_{t-1} + W_{s} s_{t} + b) - h_{t-1}, 0_{h}, -s_{t}, -\delta_{t}, 0, 0_{\omega}, -\|s_{t}\|, 0_{\omega}] \]

and hence
\[ z_{t}^{(2)} = O^{(2)}(\alpha_{t}^{(2)}) + \alpha_{t}^{(2)} = [\sigma(W_{h} h_{t-1} + W_{s} s_{t} + b), 0_{h}, 0_{s}, 0_{\omega}, 1_{t}, 0_{\omega}, 0_{\omega}, 0_{\omega}, \omega_{t}], \]

which gives
\[ y_{t+1} = [h_{t}, 0_{h}, 0_{s}, 0_{\omega}, 1_{t}, 0_{\omega}, 0_{\omega}, 0_{\omega}, \omega_{t} \]

proving the induction hypothesis (14) for \( t + 1 \), and completing the simulation of RNN.
E.1 Technical Lemmas

Lemma E.2. There exists a function \( O^{(1)}(\cdot) \) defined by feed-forward network such that,

\[
O^{(1)}(a_t^{(1)}) = [0_h, 0_h, -s_{0:t}, \delta_t, \frac{1}{2^t} + \frac{1}{2^{t+1}}, 0_w, -\omega_t, -\omega_{t-1} + \omega_t]
\]

Proof. We define the feed-forward network \( O^{(1)}(\cdot) \) such that

\[
O^{(1)}(a_t^{(1)}) = [0_h, 0_h, -s_{0:t}, \delta_t - \omega_t, \frac{1}{2^t} + \frac{1}{2^{t+1}}, 0_w, 0_w, -\omega_{t-1} + \omega_t]
\]

where

\[
\delta_t = (\Delta_{t,1}, \ldots, \Delta_{t,n-1,1/2^{t+1}}, 0 \leq \delta_t \leq 1)
\]

Recall that,

\[
a_t^{(1)} = [h_{t-1}, 0_h, s_{0:t}, \omega_t, \frac{1}{2^t}, 0_w, 0_w, \omega_{t-1}]
\]

We define the feed-forward network \( O(a_t) \) as follows,

\[
O^{(1)}(a_t) = W_2 \sigma(W_1 a_t^{(1)} + b_1)
\]

where \( W_1 \in \mathbb{Q}^{d \times d} \) and \( b_1 \in \mathbb{Q}^d \). Define \( W_1 \) as

\[
\begin{bmatrix}
2d_h & d_e & d_{\omega} & 1 & d_w & d_{\omega} & d_{\omega} \\
2d_h & 0 & 0 & 0 & 0 & 0 & 0 \\
d_e & 0 & 1 & 0 & 0 & 0 & 0 \\
d_{\omega} - 1 & 0 & 0 & 0 & 0 & 1 & -1 \\
1 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\
d_w & 0 & 0 & 1 & 0 & 0 & 0 \\
d_{\omega} & 0 & 0 & 0 & 0 & 1 & 0 \\
d_{\omega} & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\]

and \( b_1 = 0 \), then

\[
\sigma(W_1 a_t^{(1)} + b_1) = [0_h, 0_h, s_{0:t}, \Delta_t, \frac{1}{2^t+1}, \omega_t, \omega_{t-1}, \omega_{t-1}]
\]

We define \( W_2 \) as

\[
\begin{bmatrix}
2d_h & d_e & d_{\omega} - 1 & 2 & d_w & d_{\omega} & d_{\omega} \\
2d_h & 0 & 0 & 0 & 0 & 0 & 0 \\
d_e & 0 & -1 & 0 & 0 & 0 & 0 \\
d_{\omega} - 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 1,0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & -2,1 & 0 & 0 \\
d_w & 0 & 0 & 1 & 0 & 0 & 0 \\
d_{\omega} & 0 & 0 & 0 & 0 & -1 & 0 \\
d_{\omega} & 0 & 0 & 0 & 0 & 0 & -1
\end{bmatrix}
\]
This leads to
\[
O^{(1)}(\alpha^{(1)}_t) = \begin{bmatrix}
0_h, 0_h, s_{0:t}, \delta_t, \\
0_h, 0_h, s_{0:t}, -\omega_t, -\omega_{t-1} + \omega_t
\end{bmatrix}
\]

which is what we wanted to prove.

\[\square\]

**Lemma E.3.** Let \( p^{(2)}_t \in \mathbb{Q}^d \) be a query vector such that
\[
p^{(2)}_t = \begin{bmatrix}
\delta_t, \\
\cdot, \cdot, \cdot
\end{bmatrix}
\]
where \( t \geq 0 \) and \( \cdot \) denotes an arbitrary value. Then we have
\[
\text{Att}(p^{(2)}_t, K^e_{i}, V^e_{i}) = \begin{bmatrix}
0_h, 0_h, s_{t}, \\
0_h, 0_h, s_{t}, -\omega_t, -\omega_{t-1} + \omega_t
\end{bmatrix}
\]

\[(16)\]

**Proof.** Let
\[
(\hat{\alpha}^{(2,2)}_{t,1}, \ldots, \hat{\alpha}^{(2,2)}_{t,t}) = \text{hardmax} \left( \langle p^{(2)}_t, K^e_{1} \rangle, \ldots, \langle p^{(2)}_t, K^e_{t} \rangle \right)
\]
be the vector of normalized attention scores in the decoder-encoder attention block of layer 2 at time \( t \). Then
\[
\text{Att}(p^{(2)}_t, K^e_{i}, V^e_{i}) = \sum_{j=0}^{t} \hat{\alpha}^{(2,2)}_{t,j} v^e_j.
\]

We claim that

**Claim 1.** For \( t \geq 0 \) we have
\[
(\hat{\alpha}^{(2,2)}_{t,1}, \ldots, \hat{\alpha}^{(2,2)}_{t,t}) = \frac{1}{\lambda_{t}} \left( \mathbb{I}(s_0 = s_t), \mathbb{I}(s_1 = s_t), \ldots, \mathbb{I}(s_{t} = s_t) \right),
\]
where \( \lambda_{t} \) is a normalization factor given by
\[
\lambda_{t} = \sum_{j=0}^{n-1} \mathbb{I}(s_j = s_t).
\]

We now prove the lemma assuming the claim above. Denote the L.H.S. in (16) by \( \gamma_t \). Note that if \( s_j = s_t \), then \( v^e_j = \gamma_t \). Now we have
\[
\sum_{j=0}^{t} \hat{\alpha}^{(2,2)}_{t,j} v^e_j = \frac{1}{\lambda_{t}} \sum_{j=0}^{t} \mathbb{I}(s_j = s_t) v^e_j
\]
\[
= \frac{1}{\lambda_{t}} \left( \sum_{j=0}^{t} \mathbb{I}(s_j = s_t) \right) \gamma_t
\]
\[
= \gamma_t,
\]
completing the proof of the lemma modulo the proof of the claim, which we prove next.

\[\square\]
Proof. (of Claim 1) For $0 < t \leq n$, the vector $\omega_t - \omega_{t-1}$ has the form

$$
\left( \left( \frac{1}{t+1} - \frac{1}{t} \right), \ldots, \left( \frac{\phi_{t,k} - \phi_{t-1,k}}{t+1} \right), \ldots, 0 \right).
$$

If $s_t = \beta_k$, then

$$
\begin{align*}
(\omega_t - \omega_{t-1})_k &= \left( \frac{\phi_{t,k} - \phi_{t-1,k}}{t+1} \right) \\
&= \left( \frac{\phi_{t-1,k} + 1}{t+1} - \frac{\phi_{t-1,k}}{t} \right) \\
&= \frac{t - \phi_{t-1,k}}{t(t+1)} \\
&\geq \frac{1}{t(t+1)}.
\end{align*}
$$

The last inequality used our assumption that $s_0 = \#$ and that $\#$ does not occur at any later time and therefore $\phi_{t-1,j} < t$. On the other hand, if $s_t \neq \beta_k$, then

$$
\begin{align*}
(\omega_t - \omega_{t-1})_k &= \left( \frac{\phi_{t,k} - \phi_{t-1,k}}{t+1} \right) \\
&= \left( \frac{\phi_{t-1,k} + 1}{t+1} - \frac{\phi_{t-1,k}}{t} \right) \\
&= \frac{-\phi_{t-1,j}}{t(t+1)} \\
&\leq 0.
\end{align*}
$$

This leads to,

$$(\omega_t - \omega_{t-1})_k > 0 \quad \text{if } s_t = \beta_k,$$

$$(\omega_t - \omega_{t-1})_k \leq 0 \quad \text{otherwise.}$$

In words, the change in the proportion of a symbol is positive from step $t - 1$ to $t$ if and only if it is the input symbol at the $t$-th step. For $0 \leq t \leq n$ and $1 \leq k \leq |\Sigma|$, this leads to

$$
\begin{align*}
\Delta_{t,k} &= \sigma(\omega_t - \omega_{t-1})_k > 0 \quad \text{if } s_t = \beta_k, \\
\Delta_{t,k} &= \sigma(\omega_t - \omega_{t-1})_k = 0 \quad \text{otherwise},
\end{align*}
$$

For $t > n$,

$$\Delta_t = 0.$$

Recall that $p_i^{(2)} = z_i^{(1)}$ which comes from (15), and $k_j^c$ is defined in (13). We reproduce these for convenience:

$$
p_i^{(2)} = \left[ \begin{array}{cccc}
h_{t-1}, & 0_h, & 0_s, & 0_w, \\
\frac{1}{t+1}, & 0, & 0_w, & 0_w, \\
\frac{1}{t+1}, & 0, & 0_w, & 0_w, \\
\phi_t, & 0_h, & 0_s, & 0_w, \\
\end{array} \right],
$$

$$
k_j^c = \left[ \begin{array}{cccc}
h, & 0_h, & 0_s, & 0_w, \\
\frac{1}{t+1}, & 0, & 0_w, & 0_w, \\
\frac{1}{t+1}, & 0, & 0_w, & 0_w, \\
[s_j], & 0, & 0_w, & 0_w, \\
\end{array} \right].
$$

It now follows that for $0 < t < n$, if $0 \leq j \leq t$ is such that $s_j \neq s_t$, then

$$
\langle p_i^{(2)}, k_j^c \rangle = \langle \delta_t, [s_j] \rangle = \delta_{t,i} = 0.
$$
And for $0 < t < n$, if $0 \leq j \leq t$ is such that $s_j = s_t = \beta_i$, then

$$\langle p^{(2)}_t, k^o_j \rangle = \langle \delta_t, \llbracket s_j \rrbracket \rangle = \delta_{t,i}$$

(23)

$$= \frac{t - \phi_{t-1,j}}{t(t+1)} \geq \frac{1}{t(t+1)}.$$  \hspace{1cm} (24)

Thus, for $0 \leq t < n$, in the vector $\left( \langle p^{(2)}_t, k^o_0 \rangle, \ldots, \langle p^{(2)}_t, k^o_t \rangle \right)$, the largest coordinates are the ones indexed by $j$ with $s_j = s_t$ and they all equal $\frac{t - \phi_{t-1,j}}{t(t+1)}$. All other coordinates are 0. For $t \geq n$, only the last coordinate $\langle p^{(2)}_t, k^o_n \rangle = \langle \delta_t, \llbracket s \rrbracket \rangle = \frac{1}{2n+2}$ is non-zero. Now the claim follows immediately by the definition of hardmax.

\[\square\]

**Lemma E.4.** There exists a function $O^{(2)}(.)$ defined by feed-forward network such that, for $t \geq 0$,

$$O^{(2)}(a^{(2)}_t) = \left[ \sigma(W_h h_{t-1} + W_x s_t + b) - h_{t-1},
0_h, -s_t, -\delta_t, 0, 0_o, -\llbracket s \rrbracket, 0_o \right]$$

where $W_h, W_x$ and $b$ denote the parameters of the RNN under consideration.

\[\square\]

**Proof.** Proof is very similar to proof of lemma D.3.

\[\square\]

### F  Details of Experiments

In this section, we describe the specifics of our experimental setup. This includes details about the dataset, models, setup and some sample outputs.

**F.1  Impact of Residual Connections**

The models under consideration are the vanilla Transformer, the one without decoder-encoder residual connection and the one without decoder-decoder residual connection. For the copy task we random sample sentences from the Penn Treebank of lengths between 5-12 words. The train-test split is 40k-1k. All three models could easily perform this task with a network of single layer encoder and decoder with only a single attention head in each block.

For the counting task, we generate a very simple dataset where the inputs are numbers 0 to 100 and the outputs are the next 5 numbers. Here our goal is not to see whether the model will generalize to new data but to investigate whether the model is even capable of learning this task itself. Our hypothesis is that the model without decoder-encoder residual connection is incapable of learning it regardless of the size of training data or the size of the model. On the other hand both the vanilla and the one without decoder-decoder residual connections are capable but we check whether they able to learn to do it in practice. That is to learn to make inferences solely based on previous computations since there is only a single input. Our results show that they are able to perform it with only a single layer encoder-decoder network and with only a single attention head. Refer to Table 3 for a sample output.

Our implementation of the Transformer is adapted from the implementation of [20].

| Source | Reference |
|--------|-----------|
| -      | - 42      |
| Reference | - 43 44 45 46 47 |

| VANILLA TRANSFORMER | - 43 44 45 46 47 |
| Dec-Enc Residual   | - 27 27 27 27 27 |
| Dec-Dec Residual   | - 43 44 45 46 47 |

Table 3: Sample outputs by the models on the counting task. Without the residual connection around Decoder-Encoder block, the model is incapable of predicting more than one distinct output.
Table 4: Sample outputs by the models on the copy task on length 16. With absolute positional encodings the model overfits on terminal symbol at position 13 and generates sequence of length 12.

For the machine translation task we consider two datasets namely the IWSLT14 German-English dataset and IWSLT 15 English-Vietnamese dataset. We use OpenNMT [10] for our MT experiments. For preprocessing the German-English dataset we used the script from fairseq. The dataset contains about 153k training sentences, 7k development sentences and 7k test sentences. The hyperparameters to train the vanilla Transformer were obtained from fairseq’s guidelines. We tuned the parameters on the validation set for the two baseline model. To preprocess the English-Vietnamese dataset, we follow [14]. The dataset contains about 133k training sentences. We use the tst2012 dataset containing 1.5k sentences for validation and tst2013 containing 1.3k sentences as test set. We use noam optimizer in all our experiments. While tuning the network, we vary the number of layer from 1 to 6, the learning rate, the number of heads, the warmup steps, embedding size and feedforward embedding size.

F.2 Masking and Encodings

For evaluating the generalization of the models with positional masking or encoding, we simply extend the copy task up to higher lengths. The training set remains the same as before containing sentences of lengths 5-12 words. We create 5 different validation sets each containing 1k sentences each. The first set contains sentences within the same length as seen in training (5-12), the second set contains sentences of length 13 to 15 words, the third 16-20, the fourth contains sentences of length 21 to 25 and the 5th contains sentences of length 26 to 30 words. The second validation set is just there to test across a smaller variation (1-3 extra words) and then each split increases by 5 words. Our implementation for directional transformer is based on [34] but we use only unidirectional masking as opposed to bidirectional used in their setup. While tuning the models, we vary the layers from 1 to 4, the learning rate, warmup steps and the number of heads.