ODE Transformer: An Ordinary Differential Equation-Inspired Model for Neural Machine Translation

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Abstract

It has been found that residual networks are an Euler discretization of solutions to Ordinary Differential Equations (ODEs). In this paper, we explore a deeper relationship between Transformer and numerical methods of ODEs. We show that a residual block of layers in Transformer can be described as a higher-order solution to ODEs. This leads us to design a new architecture (call it ODE Transformer) analogous to the Runge-Kutta method that is well motivated in ODEs. As a natural extension to Transformer, ODE Transformer is easy to implement and parameter efficient. Our experiments on three WMT tasks demonstrate the genericity of this model, and large improvements in performance over several strong baselines. It achieves 30.76 and 44.11 BLEU scores on the WMT'14 En-De and En-Fr test data. This sets a new state-of-the-art on the WMT'14 En-Fr task.

1 Introduction

Residual networks have been used with a great success as a standard method of easing information flow in multi-layer neural models (He et al., 2016; Vaswani et al., 2017). Given an input $y_t$, models of this kind define the output of a layer at depth $t$ to be:

$$y_{t+1} = y_t + F(y_t, \theta_t)$$ (1)

where $F(\cdot, \cdot)$ is the function of the layer and $\theta_t$ is its parameter. Interestingly, recent work in machine learning (Weinan, 2017; Lu et al., 2018; Haber et al., 2018; Chang et al., 2018; Ruthotto and Haber, 2019) points out that Eq. (1) is an Euler discretization of the Ordinary Differential Equation (ODE), like this:

$$\frac{dy(t)}{dt} = F(y(t), \theta(t))$$ (2)

where $y(t)$ and $\theta(t)$ are continuous with respect to $t$. In this way, we can call Eq. (1) an ODE block. This finding offers a new way of explaining residual networks in the view of numerical algorithms. Then, one can think of a multi-layer network as applying the Euler method (i.e., Eq. (1)) to solve Eq. (2) subject to the initial conditions $y(0) = y_0$ and $\theta(0) = \theta_0$.

The solution of Eq. (2) has a sufficiently low error bound (call it a stable solution) only if $\theta(t)$ changes slow along $t$ (Haber and Ruthotto, 2017; Chen et al., 2018). But this assumption does not always hold for state-of-the-art natural language processing (NLP) systems, in which models are non-linear and over-parameterized. For example, language modeling and machine translation systems learn quite different parameters for different layers, especially when the layers are close to the model input (Vaswani et al., 2017; Dai et al., 2019). Also, truncation errors are nonnegligible for the Euler method because it is a first-order approximation to the true solution (He et al., 2019). These problems make the situation worse, when more layers are stacked and errors are propagated through the neural network. It might explain why recent Machine Translation (MT) systems cannot benefit from extremely deep models (Wang et al., 2019; Liu et al., 2020; Wei et al., 2020; Li et al., 2020).

In this paper we continue the line of research on the ODE-inspired method. The basic idea is to use a high-order method for more accurate numerical solutions to the ODE. This leads to a larger ODE block that generates a sequence of intermediate approximations to the solution. We find that the larger ODE block is sufficient to take the role of several ODE blocks with first-order solutions. The benefit
We start with a description of Transformer, followed by its relationship with ODEs. We choose Transformer for our discussion and experiments because it is one of the state-of-the-art models in recent MT evaluations.

2.1 Transformer

Transformer is an example of the encoder-decoder paradigm (Vaswani et al., 2017). The encoder is a stack of identical layers. Each layer consists of a self-attention block and a feedforward network (FFN) block. Both of them equip with a residual connection and a layer normalization unit. Note that the term “block” is used in many different ways. In this paper, the term refers to any neural network that is enhanced by the residual connection (occasionally call it a residual block).

Following the Pre-norm architecture (Wang et al., 2019), we define a block as

\[ y_{t+1} = y_t + G(LN(y_t), \theta_t) \]  

where LN(⋅) is the layer normalization function\(^1\), and \(G(⋅)\) is either the self-attention or feedforward network. \(\theta_t\) is the model parameter of the block.  

In this paper, the term refers to any neural network that is enhanced by the residual connection. In one-dimensional problems (Wang et al., 2019), we define a block as

\[ \text{ODE Block} \]

\[ \theta_1 \]

\[ \theta_2 \]

\[ \theta_3 \]

\[ \theta_4 \]

\[ \theta_5 \]

\[ \theta_6 \]

6 ODE blocks with 1st-order solutions

2 ODE blocks with 3rd-order solutions

Figure 1: Models with different ODE blocks.

is obvious: the use of fewer ODE blocks lowers the risk of introducing errors in block switching, and the high-order method reduces the approximation error in each ODE block. See Figure 1 for a comparison of different models.

Our method is parameter-efficient because \(\theta(t)\) is re-used within the same ODE block. As another “bonus”, the model can be improved by learning coefficients of different intermediate approximations in a block. We evaluate our method in strong Transformer systems, covering both the wide (and big) model and the deep model. It achieves 30.76 and 44.11 BLEU scores on the WMT14 En-De and En-Fr test sets. This result sets a new state-of-the-art in Trans-former and ODEs

2.2 Ordinary Differential Equations

An ordinary differential equation is an equation involving a function \(y(t)\) of a variable \(t\) and its derivatives. A simple form of ODE is an equation that defines the first-order derivative of \(y(t)\), like this

\[ \frac{dy(t)}{dt} = f(y(t), t) \]  

where \(f(y(t), t)\) defines a time-dependent vector field if we know its value at all points of \(y\) and all instants of time \(t\). Eq. (4) covers a broad range of problems, in that the change of a variable is determined by its current value and a time variable \(t\).

This formulation also works with Pre-norm Transformer blocks. For notational simplicity, we re-define \(G(LN(y_t), \theta_t)\) as a new function \(F(y_t, \theta_t)\):

\[ F(y_t, \theta_t) = G(LN(y_t), \theta_t) \]  

We then relax \(y_t\) and \(\theta_t\) to continuous functions \(y(t)\) and \(\theta(t)\), and rewrite Eq. (3) to be:

\[ y(t + \Delta t) = y(t) + \Delta t \cdot F(y(t), \theta(t)) \]

where \(\Delta t\) is the change of \(t\), and is general called step size. Obviously, we have \(\Delta t = 1\) in Transformer. But we can adjust step size \(\Delta t\) using a limit, and have

\[ \lim_{\Delta t \to 0} \frac{y(t + \Delta t) - y(t)}{\Delta t} = F(y(t), \theta(t)) \]  

Given the fact that \(\lim_{\Delta t \to 0} \frac{y(t + \Delta t) - y(t)}{\Delta t} = \frac{dy(t)}{dt}\), Eq. (7) is an instance of Eq. (4). The only

\(^1\)We drop the parameter of LN(⋅) for simplicity.
difference lies in that we introduce $\theta(t)$ into the right-hand side of Eq. (4).

Then, we say that a Pre-norm Transformer block describes an ODE. It has been found that Eq. (3) shares the same form as the Euler method of solving the ODE described in Eq. (7) (Haber and Ruthotto, 2017). This establishes a relationship between Transformer and ODEs, in that, given $F(t, \cdot)$ and learned parameters $\{\theta_t\}$, the forward pass of a multi-block Transformer is a process of running the Euler method for several steps.

3 The ODE Transformer

In numerical methods of ODEs, we want to ensure the precise solutions to the ODEs in a minimum number of computation steps. But the Euler method is not “precise” because it is a first-order method, and naturally with local truncation errors. The global error might be larger if we run it for a number of times\(^2\). This is obviously the case for Transformer, especially when the multi-layer neural network arises a higher risk of unstability in solving the ODEs (Haber and Ruthotto, 2017).

3.1 High-Order ODE Solvers

Here we use the Runge-Kutta methods for a higher order solution to ODEs (Runge, 1895; Kutta, 1901; Butcher, 1996; Ascher and Petzold, 1998). They are a classic family of iterative methods with different orders of precision\(^3\). More formally, the explicit Runge-Kutta methods of an $n$-step solution is defined to be:

\[
y_{t+1} = y_t + \sum_{i=1}^{n} \gamma_i F_i \\
F_1 = hf(y_t, t) \\
F_i = hf(y_t + \sum_{j=1}^{i-1} \beta_{ij} F_j, t + \alpha_i h) \\
\]

where $h$ is the step size and could be simply 1 in most cases. $F_i$ is an intermediate approximation to the solution at step $t + \alpha_i h$. $\alpha, \beta$ and $\gamma$ are coefficients which can be determined by the Taylor series of $y_{t+1}$ (Butcher, 1963). Eq. (10) describes a sequence of solution approximations $\{F_1, ..., F_n\}$ over $n$ steps $\{t + \alpha_1 h, ..., t + \alpha_n h\}$. These approximations are then interpolated to form the final solution, as in Eq. (8).

The Runge-Kutta methods are straightforwardly applicable to the design of a Transformer block. All we need is to replace the function $f$ (see Eq. (10)) with the function $F$ (see Eq. (5)). The advantage is that the function $F$ is re-used in a block. Also, the model parameter $\theta_t$ can be shared within the block\(^4\). In this way, one can omit $t + \alpha_i h$ in Eq. (10), and compute $F_i$ by

\[
F_i = F(y_t + \sum_{j=1}^{i-1} \beta_{ij} F_j, \theta_t) \\
\]

This makes the system more parameter-efficient. As would be shown in our experiments, the high-order Runge-Kutta methods can learn strong NMT systems with significantly smaller models.

The Runge-Kutta methods are general. For example, the Euler method is a first-order instance of them. For a second-order Runge-Kutta (RK2) block, we have

\[
y_{t+1} = y_t + \frac{1}{2} (F_1 + F_2) \\
F_1 = F(y_t, \theta_t) \\
F_2 = F(y_t + F_1, \theta_t) \\
\]

This is also known as the improved Euler method. Likewise, we can define a fourth-order Runge-Kutta (RK4) block to be:

\[
y_{t+1} = y_t + \frac{1}{6} (F_1 + 2F_2 + 2F_3 + F_4) \\
F_1 = F(y_t, \theta_t) \\
F_2 = F(y_t + \frac{1}{2} F_1, \theta_t) \\
F_3 = F(y_t + \frac{1}{2} F_2, \theta_t) \\
F_4 = F(y_t + F_3, \theta_t) \\
\]

See Figure 2 for a comparison of different Runge-Kutta blocks. It should be noted that the method presented here can be interpreted from

\(^2\)The global error is what we would ordinarily call the error: the difference between $y(t)$ and the true solution. The local error is the error introduced in a single step: the difference between $y(t)$ and the solution obtained by assuming that $y(t - 1)$ is the true solution.

\(^3\)A $p$-order numerical method means that the global truncation error is proportional to $p$ power of the step size.

\(^4\)Although we could distinguish the parameters at different steps in a block, we found that it did not help and made the model difficult to learn.
the perspective of representation refinement (Greff et al., 2017). It provides a way for a function to update the function itself. For example, Universal Transformer refines the representation of the input sequence using the same function and the same parameters in a block-wise manner (Dehghani et al., 2019). Here we show that inner block refinements can be modeled with a good theoretical support.

3.2 Coefficient Learning

In our preliminary experiments, the RK2 and RK4 methods yielded promising BLEU improvements when the model was shallow. But it was found that the improvement did not persist for deeper models. To figure out why this happened, let us review the Runge-Kutta methods from the angle of training. Take the RK2 method as an example. We rewrite Eq. (12) by substituting $F_1$ and $F_2$, as follow

$$y_{t+1} = y_t + \frac{1}{2} F(y_t, \theta_t) + \frac{1}{2} F(y_t + F(y_t, \theta_t), \theta_t)$$  \hspace{1cm} (20)

Let $E$ be the loss of training, $L$ be the number blocks of the model, and $y_L$ be the model output. The gradient of $E$ at $y_t$ is

$$\frac{\partial E}{\partial y_t} = \frac{\partial E}{\partial y_L} \cdot \frac{1}{2^{L-1}} \cdot \prod_{k=t}^{L-1} (1 + g_k)$$ \hspace{1cm} (21)

where

$$g_k = \left(1 + \frac{\partial F(y_k, \theta_k)}{\partial y_k}\right) \cdot \left(1 + \frac{\partial F(y_k + F(y_k, \theta_k), \theta_k)}{\partial y_k + F(y_k, \theta_k)}\right)$$  \hspace{1cm} (22)

Seen from Eq. (29), $\frac{\partial E}{\partial y_t}$ is proportional to the factor $\frac{1}{2^{L-t}}$. This leads to a higher risk of gradient vanishing when $L$ is larger.

The problem somehow attributes to the small coefficients of $F_i$, that is, $\gamma_1 = \gamma_2 = \frac{1}{2}$. A natural idea is to empirically set $\gamma_i = 1$ to eliminate the product factor of less than 1 in gradient computation, although this is not theoretically grounded in standard Runge-Kutta methods. We rewrite Eq. (20) with the new coefficients, as follows

$$y_{t+1} = y_t + F(y_t, \theta_t) + F(y_t + F(y_t, \theta_t), \theta_t)$$ \hspace{1cm} (23)

Then, we have the gradient, like this

$$\frac{\partial E}{\partial y_t} = \frac{\partial E}{\partial y_L} \prod_{k=t}^{L-1} g_k$$ \hspace{1cm} (24)

This model is easy to optimize because $\frac{\partial E}{\partial y_L}$ can be passed to lower-level blocks with no scales. Note that, the methods here are instances of parameter sharing (Dehghani et al., 2019). For example, in each ODE block, we use the same function $F$ with the same parameter $\theta_t$ for all intermediate steps. Setting $\gamma_i = 1$ is a further step towards this because $F_i$ is passed to next steps with the same scale. Here we call it implicit parameter sharing.

Another method of scaling $F_i$ is to learn the coefficients automatically on the training data (with the initial value $\gamma_i = 1$). It helps the system learn the way of flowing $F_i$ in a block. Our experiments show that the automatic coefficient learning is necessary for better results (see Section 4).

Figure 2: Architectures of ODE Transformer blocks.
Table 1: Comparison with the state-of-the-arts on WMT En-De and WMT En-Fr tasks. We both report the tokenized BLEU and sacrebleu scores for comparison with previous work.

| Model                          | Layers | WMT En-De | WMT En-Fr |
|-------------------------------|--------|-----------|-----------|
|                               |        | #Param | Steps | BLEU | SBLEU | #Param | Steps | BLEU | SBLEU |
| Vaswani et al. (2017) - Transformer | 6-6    | 213M | 100K | 28.40 | - | 222M | 300K | 41.00 | - |
| Ott et al. (2018) - Scaling NMT | 6-6    | 210M | 100K | 29.30 | 28.6 | 222M | 100K | 43.20 | 41.4 |
| Dehghani et al. (2019) - Universal Transformer | - | - | - | 28.90 | - | - | - | - | - |
| Lu et al. (2019) - MacaronNet | 6-6    | - | - | 30.20 | - | - | - | - | - |
| Fan et al. (2020) - LayerDrop | 12-6   | 286M | 100K | 30.20 | - | - | - | - | - |
| Wu et al. (2019) - Depth growing | 8-8    | 270M | 800K | 29.92 | - | - | - | - | 43.27 |
| Wang et al. (2019) - Transformer-DLCL | 30-6   | 137M | 50K | 29.30 | 28.6 | 100M | 300K | 43.20 | 41.4 |
| Ott et al. (2018) - Scaling NMT | 6-6    | 210M | 100K | 29.30 | 28.6 | 222M | 100K | 43.20 | 41.4 |
| Dehghani et al. (2019) - Universal Transformer | - | - | - | 28.90 | - | - | - | - | - |
| Lu et al. (2019) - MacaronNet | 6-6    | - | - | 30.20 | - | - | - | - | - |
| Fan et al. (2020) - LayerDrop | 12-6   | 286M | 100K | 30.20 | - | - | - | - | - |
| Wu et al. (2019) - Depth growing | 8-8    | 270M | 800K | 29.92 | - | - | - | - | 43.27 |
| Wang et al. (2019) - Transformer-DLCL | 30-6   | 137M | 50K | 29.30 | 28.6 | 100M | 300K | 43.20 | 41.4 |
| Ott et al. (2018) - Scaling NMT | 6-6    | 210M | 100K | 29.30 | 28.6 | 222M | 100K | 43.20 | 41.4 |
| Dehghani et al. (2019) - Universal Transformer | - | - | - | 28.90 | - | - | - | - | - |
| Lu et al. (2019) - MacaronNet | 6-6    | - | - | 30.20 | - | - | - | - | - |
| Fan et al. (2020) - LayerDrop | 12-6   | 286M | 100K | 30.20 | - | - | - | - | - |
| Wu et al. (2019) - Depth growing | 8-8    | 270M | 800K | 29.92 | - | - | - | - | 43.27 |
| Wang et al. (2019) - Transformer-DLCL | 30-6   | 137M | 50K | 29.30 | 28.6 | 100M | 300K | 43.20 | 41.4 |
| Ott et al. (2018) - Scaling NMT | 6-6    | 210M | 100K | 29.30 | 28.6 | 222M | 100K | 43.20 | 41.4 |
| Dehghani et al. (2019) - Universal Transformer | - | - | - | 28.90 | - | - | - | - | - |
| Lu et al. (2019) - MacaronNet | 6-6    | - | - | 30.20 | - | - | - | - | - |
| Fan et al. (2020) - LayerDrop | 12-6   | 286M | 100K | 30.20 | - | - | - | - | - |
| Wu et al. (2019) - Depth growing | 8-8    | 270M | 800K | 29.92 | - | - | - | - | 43.27 |
| Wang et al. (2019) - Transformer-DLCL | 30-6   | 137M | 50K | 29.30 | 28.6 | 100M | 300K | 43.20 | 41.4 |

4 Experiments

4.1 Experimental Setups

Our proposed methods were evaluated on three widely-used benchmarks: the WMT’14 English-German (En-De), WMT’14 English-French (En-Fr) and WMT’16 English-Romanian (En-Ro) translation tasks.

Datasets and Evaluations: For the En-De task, the training data consisted of approximately 4.5M tokenized sentence pairs, as in (Vaswani et al., 2017). All sentences were segmented into sequences of sub-word units (Sennrich et al., 2016) with 32K merge operations using a shared vocabulary. We selected newstest2013 as the validation data and newstest2014 as the test data. For the En-Fr task, we used the dataset provided by Fairseq, i.e., 36M training sentence pairs from WMT’14. newstest2012+newstest2013 was the validation data and newstest2014 was the test data. For the En-Ro task, we replicated the setup of (Mehta et al., 2020), which used 600K/2K/2K sentence pairs for training, evaluation and inference, respectively.

We measured performance in terms of BLEU (Papineni et al., 2002). Both tokenized BLEU scores and sacrebleu were reported on the En-De and the En-Fr tasks. Also, we report tokenized BLEU scores on the En-Ro task. The beam size and length penalty were set to 4 and 0.6 for the En-De and the En-Fr, and 5 and 1.3 for the En-Ro.

Training Details: As suggested in Li et al. (2020)’s work, we used relative positional representation (RPR) for a stronger baseline (Shaw et al., 2018). All experiments were trained on 8 GPUs, with 4,096 tokens on each GPU. For the En-De and the En-Fr tasks, we employed the gradient accumulation strategy with a step of 2 and 8, respectively. We used the Adam optimizer (Kingma and Ba, 2015) whose hyperparameters were set to (0.9, 0.997), and the max point of the learning rate was set to 0.002 for fast convergence. We regard merging SAN and FFN as the default ODE block. More details could be found in our supplementary materials.

5 Computed by multi-bleu.perl
6 BLEU+case.mixed+numrefs.1+smooth.exp+tok.13a+version.1.2.12
Table 2: Results on the WMT En-Ro task. † indicates the related information is not reported.

Table 3: The comparison of model efficiency on the WMT En-De task.

### 4.2 Results

**Results of En-De and En-Fr:** Table 1 compares ODE Transformer with several state-of-the-art systems. Both RK2-block and RK4-block outperform the baselines by a large margin with different model capacities. For example, RK2-block obtains a 0.97 BLEU improvement with the base configuration when the depth is 6. RK4-block yields a gain of +0.17 BLEU points on top of RK2-block. This observation empirically validates the conjecture that high-order ODE functions are more efficient. When we switch to deep models, RK2-block is comparable with a 48-layer strong system reported in (Li et al., 2020) with significantly fewer parameters, indicating our method is parameter efficient.

Wide models can also benefit from the enlarging layer depth (Wei et al., 2020; Li et al., 2020). The RK-2 ODE Transformer achieves BLEU score of 30.76 and 44.11 on the En-De and the En-Fr tasks, significantly surpassing the standard Big model by 1.32 and 0.70 BLEU points. This sets a new state-of-the-art on these tasks with fewer parameters. Note that more results on RK4-block (learnable $\gamma_i$) will be reported.

**Results of En-Ro:** Table 2 exhibits model parameters, total training steps and BLEU scores of several strong systems on the En-Ro task. Again, ODE Transformer outperforms these baseline. As stated in (Mehta et al., 2020), they trained the model up to 170 epochs and obtained a BLEU score of 34.70 through the DeLight model. However, the observation here is quite different. The validation perplexity begins to increase after 20 epochs. Thus, our baseline is slightly inferior to theirs, but matches the result reported in Lin et al. (2020). ODE Transformer achieves even better performance with DeLight within much less training cost. For a bigger model (line 6 in Table 2), it obtains a BLEU score of 35.28.

**Parameter Efficiency:** Table 3 summaries the results of several efficient Transformer variants, including Lite Transformer (Wu et al., 2020), DeLight (Mehta et al., 2020) and a light version of the Evolved Transformer (So et al., 2019). As we expected, the proposed ODE Transformer is promising for smaller models. It is comparable in BLEU with DeLight but having 9M fewer parameters. Under the same model capacity, it outperforms DeLight by 0.84 BLEU points. These results demonstrate that the proposed method is orthogonal to the model capacity. It may offer a new choice for deploying NMT systems on edge devices.

### 4.3 Analysis

Here we investigate some interesting issues. For simplicity, in the following, we call RK2-block with learnable coefficients as RK2-block-v2.

**BLEU against Encoder Depth:** Figure 3 (left) depicts BLEU scores of several ODE Transformer variants and the baseline under different encoder depths. All ODE Transformer variants are significantly superior to the baseline when the depth $\leq 24$. And the RK2-block-v2 almost achieves the best performance over all depths, especially when the model becomes deeper. Intuitively, a 6-layer RK2-block is able to deliver comparable performance compared with the 18-layer baseline system. Again, it indicates the proposed method is parameter efficient. Another finding here is RK4-block behaves strongly on shallow models, similar phenomena are observed in Table 1. It is inferior to RK2-block for deeper models, though high-order ODE solvers can obtain lower errors. This is due to original coefficients may cause the optimization problem in the backward propagation when the model is deep (see Section 3.2). Also, Figure 3 (right) plots BLEU as a function of the model size when the hidden size is 256. Our RK2 method significantly surpasses the baseline using much fewer parameters.
we collect the gradient norm of several well-trained systems during training. Figure 6 plots the gradient norm of RK2-block, RK4-block and the standard residual-block (baseline). As we can see that RK2-block presents lower training and validation perplexity (PPL) in both configurations. Intuitively, RK2-block presents lower training and validation PPLs in both configurations. Here, we re-implement these methods using the same codebase for fair comparisons. We set the encoder depth as 6 following the base configuration and conducted experiments on the En-De task.

At time $t$, Multistep Euler methods requires previous states, e.g. $y_{t-1}$, to generate the current approximation, instead of iterative refinements based on the current-time state. Basically, these methods are not parameter efficient, and obtain inferior performance than ours. Note that DLCL can also be regarded as a multistep Euler method, which is more competitive in deep Transformer. But there is only a small improvement upon a shallow baseline. Theoretically, the Backward Euler method is only a small improvement upon a shallow baseline. Therefore, it is only a small improvement upon a shallow baseline. However, it is still considered a competitive method in deep Transformer. But there is only a small improvement upon a shallow baseline.

### Ablation Study on Different $F(\cdot, \cdot)$: As we stated, the $F(\cdot, \cdot)$ function can either be the sub-layer, e.g. SAN, FFN or both of them (SAN+FFN). As shown in Figure 4, high-order ODE works better with FFN than SAN. An exploration might be that the FFN component has more parameters than the SAN component$^7$. The model that merging FFN and SAN as an ODE block shows the best performance.

### Training and Validation Perplexity: Figure 5 plots the training and validation perplexity (PPL) curves of RK blocks and the standard residual-block. We compare the behaviors based on two configurations (base and wide models). Intuitively, RK2-block presents lower training and validation PPLs in both configurations.

### Visualization of the Gradient Norm: To study the superiority of the proposed ODE Transformer, we collect the gradient norm of several well-trained systems during training. Figure 6 plots the gradient norm of RK2-block, RK4-block and the standard residual-block (baseline). As we can see that Pre-Norm residual block is able to make the training stable (Wang et al., 2019). Both RK2-block and RK4-block provide richer signals due to the implicit parameter sharing among intermediate approximations. And the two learning curves likewise appear to be nearly the same, which is consistent

$^7$Mostly, there are $2 \cdot d_{\text{model}} \cdot 4d_{\text{model}}$ parameters in FFN and $d_{\text{model}} \cdot 3d_{\text{model}} + d_{\text{model}} \cdot d_{\text{model}}$ in SAN.
Quantization of the Truncation Error: Here, we aim at quantifying the truncation error. However, we cannot obtain the “true” solution of each block output in NMT, because we mainly experimented on the encoder side. Instead, we experimented on the language modeling task, where the ground truth is equivalent to the truncation error without error propagations. Table 5 shows the PPL on the PTB task. All ODE Transformer variants reduce the errors significantly. RK4-order achieves the lowest PPL on both settings. In addition, a RK2-block can even obtain lower PPL than a 2-layer residual-block. The observation here again verifies our conjecture.

5 Related Work

Deep Transformer models: Recently, deep Transformer has witnessed tremendous success in machine translation. A straightforward way is to shorten the path from upper-level layers to lower-level layers thus to alleviate the gradient vanishing or exploding problems (Bapna et al., 2018; Wang et al., 2019; Wu et al., 2019; Wei et al., 2020). For deeper models, the training cost is nonnegligible. To speed up the training, an alternative way is to train a shallow model first and progressively increasing the model depth (Li et al., 2020; Dong et al., 2020).

Apart from the model architecture improvements, another way of easing the optimization is to utilize carefully designed parameter initialization strategies, such as depth-scale (Zhang et al., 2019), Lipschitz constraint (Xu et al., 2020), T-fixup (Huang et al., 2020) and ADMIN (Liu et al., 2020). Note that the ODE Transformer is orthogonal to the aforementioned methods, and we will test it on these methods in the future work.

Ordinary Differential Equations: The relationship between the ResNet and ODEs was first proposed by Weinan (2017). This brings the community a brand-new perspective on the design of effective deep architectures. Some insightful architectures (Zhang et al., 2017; Larsson et al., 2017; Lu et al., 2018; He et al., 2019) can also be interpreted from the ODE perspective. But, in nature language processing, it is still rare to see studies on designing models from the ODE perspective. Perhaps the most relevant work with us is Lu et al. (2019)’s work. They interpreted the Transformer architecture from a multi-particle dynamic system view and relocated the self-attention sandwiched into the FFN. Unlike their work, we argue that the stacked first-order ODE blocks may cause error accumulation, thus hindering the model performance. We address this issue by introducing high-order blocks, and demonstrate significant BLEU improvements.

6 Conclusions

In this paper, we have explored the relationship between Transformer and ODEs. We have proposed a new architecture (ODE Transformer) to help the model benefit from high-order ODE solutions. Ex-
perimental results show that ODE Transformer can significantly outperform the baseline with the same model capacity. It achieves 30.76 and 44.11 BLEU scores on the WMT’14 En-De and En-Fr test data. This sets a new state-of-the-art on the En-Fr task.

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All models were trained on 8 NVIDIA TITAN V GPUs with mix-precision accelerating. And main results were the average of three times running with different random seeds. Note that we averaged the last 5/10 checkpoints for more robust results.

Since the proposed method is orthogonal to the model capacity, we evaluated the ODE Transformer on Base/Deep/Wide configurations, respectively. The detail of each configuration is as follows:

- **Base/Deep Model.** The hidden size of self-attention was 512, and the dimension of the inner-layer in FFN was 2,048. We used 8 heads for attention. For training, we set all dropout to 0.1, including residual dropout, attention dropout, ReLU dropout. Label smoothing $\epsilon_{ls} = 0.1$ was applied to enhance the generation ability of the model. For deep models, we only enlarged the encoder depth considering the inference speed.

- **Wide (or Big) Model.** We used the same architecture as Transformer-Base but with a larger hidden layer size 1,024, more attention heads (16), and a larger feed forward inner-layer (4,096 dimensions). The residual dropout was set to 0.3 for the En-De task and 0.1 for the En-Fr tasks.

### Table 6: The comparison of PPL on several systems.

| Lang    | Train | Valid | Test |
|---------|-------|-------|------|
| WMT’14 En-De | 4.5M  | 3000  | 3003 |
| WMT’14 En-Fr  | 35.7M | 26822 | 3003 |
| WMT’16 En-Ro  | 602K  | 1999  | 1999 |

In the training phase, Deep/Big models were updated for 50K and 100K steps on the En-De task, 100K steps on the En-Fr task, 17K steps on the En-Ro task.

Table 6 summarizes the details of our datasets, including the WMT En-De, the WMT En-Fr and the WMT En-Ro tasks. We both present the sentences and tokens of each task. For En-De and En-Fr task, the datasets used in this work could be found in Fairseq. For En-Ro, one can use the preprocessed dataset provided by Delight. Note that we only share the target embedding and the softmax embedding instead of a shared vocabulary between the source side and the target side.

### B Details for the PTB dataset

Here, we introduce the details about the PTB dataset and the corresponding configuration. It contains 88K, 3370 and 3761 sentences for training, validation and test. The vocabulary size was 10K. In this work, the layer depth of the language model was set to 1 or 2. The main concern here is to evaluate the truncate error. Assume the layer depth is 1, then the loss between the block output and the ground-truth can be regarded as the truncate error. It alleviates the influence of the error accumulation among different layers.

The hidden size was 512, and the filter size of the FFN was 2,048. We set all the dropout rate as 0.1, including the residual dropout, attention dropout and the relu dropout. Each model was trained up to 20 epochs, and most models achieved the lowest PPL on the validation set when the epoch is 10. Then the validation PPL began to increase, though the training PPL is still declining. The warmup-step was 2000 and the batch size was 4,096. The max learning rate was set to 0.0007. After warmup, the learning rate decayed proportionally to the inverse square root of the current step.

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8 [https://github.com/pytorch/fairseq/tree/master/examples/scaling_nmt](https://github.com/pytorch/fairseq/tree/master/examples/scaling_nmt)
9 [https://github.com/sacmehta/delight/blob/master/readme_files/nmt/wmt16_en2ro.md](https://github.com/sacmehta/delight/blob/master/readme_files/nmt/wmt16_en2ro.md)
C Derivations of the Equation

Let $\mathcal{E}$ be the loss of training, $L$ be the number blocks of the model, and $y_L$ be the model output. Here, we define

$$z_k = y_k + F(y_k, \theta_k)$$  \hfill (25)

Then the information flow of the RK2 method can be described as follows:

$$y_{k+1} = y_k + \frac{1}{2} F(y_k, \theta_k) + \frac{1}{2} F(y_k + F(y_k, \theta_k), \theta_k)$$  \hfill (26)

where $\frac{\partial z_k}{\partial y_k} = 1 + \frac{\partial F(y_k, \theta_k)}{\partial y_k}$. In this way, the detail derivation of Eq. (26) is as follows:

$$\frac{\partial y_{k+1}}{\partial y_k} = 1 + \frac{1}{2} \frac{\partial F(y_k, \theta_k)}{\partial y_k} + \frac{1}{2} \frac{\partial F(z_k, \theta_k)}{\partial z_k} \frac{\partial z_k}{\partial y_k}$$

$$= \frac{1}{2} \cdot \left( 1 + \frac{\partial F(y_k, \theta_k)}{\partial y_k} + \frac{\partial F(z_k, \theta_k)}{\partial z_k} \cdot \frac{1}{2} \frac{\partial F(z_k, \theta_k)}{\partial z_k} \right)$$

$$= \frac{1}{2} \cdot \left( 1 + \left( 1 + \frac{\partial F(z_k, \theta_k)}{\partial z_k} \right) \right) \cdot \left( 1 + \frac{\partial F(y_k, \theta_k)}{\partial y_k} \right)$$  \hfill (27)

With the chain rule, the error $\mathcal{E}$ propagates from the top layer $y_L$ to layer $y_t$ by the following formula:

$$\frac{\partial \mathcal{E}}{\partial y_t} = \frac{\partial \mathcal{E}}{\partial y_L} \cdot \frac{\partial y_L}{\partial y_{L-1}} \cdot \frac{\partial y_{L-1}}{\partial y_{L-2}} \cdots \frac{\partial y_{t+1}}{\partial y_t}$$

Here we have

$$g_k = \left( 1 + \frac{\partial F(y_k, \theta_k)}{\partial y_k} \right) \cdot \left( 1 + \frac{\partial F(z_k, \theta_k)}{\partial z_k} \right)$$  \hfill (28)

Then, put the Eq. (28) into Eq. (27), the gradient of $\mathcal{E}$ at $y_t$ is

$$\frac{\partial \mathcal{E}}{\partial y_t} = \frac{\partial \mathcal{E}}{\partial y_L} \cdot \frac{1}{2^{L-t}} \cdot \prod_{k=t}^{L-1} (1 + g_k)$$  \hfill (29)

Similarly, we can easily obtain the gradient of RK2 method where $\gamma_i = 1$: