Linear Complexity Self-Attention with $3^{rd}$ Order Polynomials

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Abstract—Self-attention mechanisms and non-local blocks have become crucial building blocks for state-of-the-art neural architectures thanks to their unparalleled ability in capturing long-range dependencies in the input. However, their cost is quadratic with the number of spatial positions, making their use impractical in many real case applications. In this work, we analyze these methods through a polynomial lens, and show that self-attention can be seen as a special case of a 3rd order polynomial. Within this polynomial framework, we are able to design polynomial operators capable of accessing the same data pattern of non-local and self-attention blocks while reducing the complexity from quadratic to linear. As a result, we propose two modules (Poly-NL and Poly-SA) that can be used as “drop-in” replacements for more-complex non-local and self-attention layers in state-of-the-art CNNs and ViT architectures. Our modules can achieve comparable, if not better, performance across a wide range of computer vision tasks while keeping a complexity equivalent to a standard linear layer.

Index Terms—self-attention, non-local blocks, transformers, polynomial expansion, neural networks

1 INTRODUCTION

CONVOLUTIONAL Neural Networks (CNNs) are often at the core of state-of-the-art methods in computer vision. However, CNNs suffer from limited receptive field, even in deep architectures, because interactions between input features decay exponentially with their distance [1].

Self-attention (SA) [2] and the non-local block (NL) [3] have been proposed as techniques to extract long-range dependencies from the input in a position-independent manner. Specifically, SA adaptively modulates any given (reference) position using contributions of all the other positions scaled by their pairwise similarity with the reference. This has been shown to be an effective strategy to enrich, or even completely replace, standard convolutional layers in a wide range of architectures and domains [4], [5], [6], [7], [8], [9], [10]. However, the effectiveness of these layers relies on computing similarities between every pair of positions. This operation has a quadratic cost (with respect to the input dimension size) and thus is prohibitive to compute when input resolution is large and/or computational resources are limited (e.g., on edge devices).

We establish a new link between the self-attention/non-local block and polynomial expansions. This new perspective enables us to design novel operators that are able to capture the same correlations as the non-local block of [3] while reducing the computational cost of these blocks from quadratic to linear without shrinking the receptive field as done in previous works [11], [12], [13].

In our preliminary work [14], we frame the NL block as a special case of $3^{rd}$ order polynomials, and introduced Poly-NL. In this work, we perform three significant extensions: a) we propose Poly-SA, a multi-head self-attention layer that extends our Poly-NL to fit Vision Transformer (ViT) architectures, which are widely used across a range of tasks [15], [10], [16]; b) We provide new insights into the link between SA/NL and the polynomial expansions (i.e. Sec. 2), as well as polynomial networks in general; c) We conduct a thorough evaluation with the newly introduced proposed Poly-SA, which highlights its ability to work as low-complexity alternative to standard attention blocks in several ViT backbones. In addition to these extensions, we d) provide additional visualizations of the long-term dependencies captured by our blocks which are able to intuitively illustrate the inner workings of our method, and e) we extend the text to discuss limitations for the interested practitioner. In summary, our contributions can be summarized as follows:

- We bridge the formulations of high-order polynomials and attention. In particular, we prove that self-attention (in the form of non-local blocks) can be seen as a particular case of general $3^{rd}$ order polynomials.
- We propose Poly-NL and Poly-SA, two novel building blocks for neural networks which can replace standard NL/SA reducing the complexity from quadratic to linear.
- We showcase the efficiency and the effectiveness of our blocks in both CNN and ViT architectures across a wide range of tasks: image recognition, instance segmentation, jigsaw puzzle reconstruction, and face detection.
2 RELATED WORK

2.1 Multiplicative Interactions

Multiplicative interactions [17], [18] are essential to various machine learning models such as LSTM, Bilinear layers, and Higher-order Boltzmann machines. In LSTM [19], [20], element-wise products are used to fuse representations. In Bilinear layers [21], [22], [23], [24] feature maps of different networks get bilinearly combined to capture pairwise interactions. In $k$th-order Boltzmann machines [25], [26], [27], $k$th order multiplicative interactions are used to define the energy function. These high order interactions capture diverse interactions between the input elements. More recently, II-nets [28] use polynomial expansions as a function approximator using tensor decompositions [29] to reduce the number of learnable parameters. A number of works have demonstrated the separation of polynomial networks from regular neural networks and their benefits with respect to expressivity [30], [17], interpretability [31], learning high frequency functions [32], and extrapolation [33].

2.2 Attention

Multiplicative interactions are also crucial in the context of self-attention. Self-attention methods have been proposed as mechanisms to self-recalibrate feature maps and have been used either as replacement or addition to traditional residual blocks [34]. Complementary to our work, some of these methods accumulate contextual information into lightweight global-descriptors extrapolating a single scalar for each spatial position [35], channel [36], [37], channel and position [38], or region of space [39]. Capturing long-range spatial dependencies among spatial positions is a long-standing problem in computer vision [40], [41], [42]. However, it had received little attention until recently in the context of neural network architectures [3], [2]. Spatial self-attention modules for neural networks leverage long-range dependencies of the input and have been used in natural language processing as well as in computer vision to achieve state-of-the-art performance in various problems such as translation [7], question answering [9], classification [8], [4], segmentation [43], [44], [45], and video processing [6], among others. Some works focused on extending the scope of attention by capturing channel correlations [46], [47], [48] or considering multiple resolutions of the image [49], [5]. Other influential works conducted in the context of architecture design proved how spatial self-attention networks (Transformers) represent a suitable alternative to CNN in vision [50], [51], [52], [53], [54].

2.3 Reducing Complexity

Despite the undisputed success of self-attention, recent works sparked a discussion on its scalability, and on how to overcome its intrinsic efficiency limitations [55]. Existing solutions focus on increasing the efficiency of the similarity operator, for example by reducing the number of positions attended [56] or using low dimensional latent spaces [57], [58]. Linear-Attention (LA) [59] replaces the softmax-attention in transformer architectures with a feature-map dot product while XCiT [60] replaces the computation of the standard attention matrix with a cross-covariance alternative. These methods linearize complexity by computing pairwise relations between features instead of spatial positions. A similar idea in the context of non-local block can be found in Double Attention network [61] and, more recently, in Efficient Attention [62]. In a similar spirit, LatentGNN [63] introduces an additional interaction operation in the latent space, representing non-local relations via a mixture of low-rank kernel matrices. Different strategies investigate alternative kernels for transformer architectures [64] and propose alternatives of linear complexity by using random features [65], [66] or kernel learning [67]. Lastly, Attention Free Transformers [68] uses element-wise multiplication to calculate attention in transformer architectures. In contrast to previous works, we propose a linear alternative of the non-local block by framing non-local dependencies as 3rd order interactions.

3 CAPTURING HIGH-ORDER INTERACTIONS IN NEURAL NETWORKS

We start by introducing notation and background, then proceed in formalizing the concept of 3rd order interactions. Our goal is to frame spatial-attention blocks and long-range interactions as a polynomial expansion.

3.1 Polynomials for Neural Networks.

We follow the notation of Kolda et al. [29]. Vectors are denoted as lower-case bold letters (e.g. $x$) and matrices as upper-case bold letters (e.g. $X$). The element at position $(i,j)$ of a matrix $X \in \mathbb{R}^{I_1 \times I_2}$ can be indicated as $x_{i,j}$. Tensors are identified with bold Euler script letters (e.g. $\mathcal{X}$). The order of a tensor is the number of dimensions, also known as way or mode. Hadamard products are indicated using the symbol “$\odot$”. Given two tensors, we define their double-dot product as the tensor contraction with respect to the last two indices of the first one and the first two indices of the second one, identified with the bullet “$\bullet$” symbol. For instance, the double-dot product between a tensor $\mathcal{W} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N \times I_N}$ and a matrix $X \in \mathbb{R}^{I_1 \times I_N}$ is a tensor of order $N - 2$, i.e. $\mathcal{Y} = \mathcal{W} \bullet X \in \mathbb{R}^{I_1 \cdots \times I_N - 2}$. Specifically, the element-wise form of the double-dot product is expressed as:

$$y_{i_1, \ldots, i_{N-2}} = \sum_{i_{n-1}=1}^{I_{n-1}} \sum_{i_{n}=1}^{I_{n}} w_{(i_1, \ldots, i_{n-2}, i_{n-1}, i_{n})} x_{(i_{n-1}, i_{n})}.$$  

In [28], the authors adopted polynomials as layers of neural networks. Intuitively each element of the output depends on all the elements of the input through a polynomial function. Formally, the output of the layer is defined as

$$Y = P(X) = \sum_{d=1}^{D} \mathcal{W}^{[d]} \prod_{j=1}^{d} \bullet X + \mathcal{W}^{[0]},$$  

where $X$ and $Y$ are the input and output matrices both having size $I_1 \times I_2$, $P$ is a polynomial function of order $D$, $\mathcal{W}^{[d]} \in \mathbb{R}^{I_1 \times I_2 \times \prod_{j=1}^{d} (I_j \times I_j)}$ is a tensor of learnable parameters associated with a specific order $d \in \{1, \ldots, D\}$, and $\mathcal{W}^{[0]}$ is a bias matrix of learnable parameters. Note that the
Fig. 1: Two views of the Poly-NL block. a) Poly-NL as a non-local self-attention block for neural networks. Gray boxes represent convolutions of kernel size 1 and an averaging function over the rows. The output of the average pooling undergoes an expansion before the Hadamard multiplication. b) Poly-NL as a 3rd order polynomial module for neural networks. In the first box the space of 3rd order interactions is represented as a line of $(NC)^3$ white dots, containing all possible triplets. The learnable parameters of $W_{Poly-NL}^{[3]} \in \mathbb{R}^{NC \times NC \times NC \times NC}$ weight each triplet $x_{(c,d)}x_{(e,f)}x_{(g,h)}$ by its importance $w_{(a,b,c,d,e,f,g,h)}$. This is depicted in the second box as a line of colored dots. The output element $y_{(a,b)}$ is the weighted summation of every triplet. Poly-NL focuses only on a small subset of all order interactions (e.g. 0.025%), which is equivalent to assuming a portion of $W_{Poly-NL}^{[3]}$ values equal to zero.

size of the parameter tensor $W^{[d]}$ increases exponentially with the order $d$ of the polynomial.

### 3.2 Higher Order Interactions

To provide some relevant background, we start by describing higher-order interactions terms for a feature map $X \in \mathbb{R}^{D \times W \times C}$, where $H$, $W$, and $C$ correspond to the height, the width and the number of channels for the given input tensor. We consider its folding $X \in \mathbb{R}^{N \times C}$, with vectorized spatial dimensions of size $N = HW$. A 2nd order polynomial building block for neural networks captures pairwise dependencies among the elements of $X$, by considering their linear combination weighted with a set of learnable parameters. The general equation for a 2nd order block can be derived by isolating the 2nd order term ($D = 2$) of Eq. (1)

$$Y = \left( \left( W^{[2]} \cdot X \right) \cdot X \right),$$

where $W^{[2]}$ is a tensor of order 6 and dimension $\mathbb{R}^{NC \times NC \times NC \times NC \times NC}$. Note that Eq. (1) acts as a generalization of a single linear layer, as visible from its element-wise equation:

$$y_{(a,b)} = \sum_{c,e}^{N} \sum_{d,f}^{C} w_{[d]} x_{(c,d)} x_{(e,f)}.$$

(3)

Analogously, to capture all 3rd order dependencies between elements of $X$, we isolate the 3rd order term ($D = 3$) of Eq. (1) by assuming $W^{[d]} = 0$ for $d \in \{0, 1, 2\}$. As a result, we obtain a simplified formulation for Eq. (1) as

$$Y = \left( \left( \left( W^{[3]} \cdot X \right) \cdot X \right) \cdot X \right).$$

(4)

where $W^{[3]}$ is a tensor of order 8 and dimension $\mathbb{R}^{NC \times NC \times NC \times NC \times NC \times NC \times NC \times NC}$. Similarly to the 2nd order case, its element-wise form is defined as

$$y_{(a,b)} = \sum_{c,e,g}^{N} \sum_{d,f,h}^{C} w_{[d]} x_{(c,d)} x_{(e,f)} x_{(g,h)},$$

(5)

which clearly highlights how Eq. (5) includes multiplication of all possible triplets of the input elements summed together, i.e., all possible 3rd order interactions. As can be seen from Eq. (5), in a 3rd order polynomial each element of the output matrix $y_{(a,b)}$ benefits from the contributions of every possible triplet $x_{(c,d)}x_{(e,f)}x_{(g,h)}$, each weighted by its unique importance $w_{[d]}$, where spatial indexes $a, c, e, g$ are ranging from 1 to $N$ and channel indexes $b, d, f, h$ are ranging from 1 to $C$. The use of $W^{[3]}$ in its most general form allows to take into account every possible interaction in the input but, at the same time, exponentially increases the number of parameters. A major issue when scaling to higher orders is the exponential growth in the number of parameters and computational cost. In our case, the number of parameters in Eq. (1) depends on the order $D$ of the polynomial and, even without considering orders lower than $D$, the parameters required are $(NC)^{D+1}$ (for instance, the use of $D = 3$ on an input $1024 \times 196$ will introduce approximately extra $10^{21}$ parameters). The number of parameters can be reduced by taking into account prior knowledge about the task or the nature of the input data [29], [26]. That is, we can select only a limited subset of all the possible combinations $x_{(c,d)}x_{(e,f)}x_{(g,h)}$ exploiting a particular structure of the tensor $W^{[3]}$. For example, assigning the same weight to a group of triplets will guarantee each of them to have same contribution on the output, while setting their weight to zero will cancel their impact altogether. The central idea of this paper is to factor the
interaction tensor $\mathbf{W}^{[3]}$ in a particular way, and extract only a minimal subset of $3^{rd}$ order interactions from the input data. Practically, we replace the interaction tensor with matrices of smaller size using efficient operators commonly used in neural networks.

## 4 Method

In this section, we formally describe the proposed non-local module, called “Poly-NL”, which is a novel operator capturing the same interactions as the non-local block [3] at a fraction of the computational cost in both space and time. Next, we adapt its formulation for Vision Transformers architectures: “Poly-SA”. Specifically, we first characterize the specific set of $3^{rd}$ order interactions associated with non-local dependencies. Then, we define a method capable of accessing them without the need to compute the expensive pairwise similarity matrix. Lastly, we align the formulation to self-attention for transformers and extend it to allow spatial adaptivity.

### 4.1 Poly-NL Layer

In [3], the authors introduce the “Non-local block”, a learnable layer used to extract long-range dependencies in the input. This block operates on a folded feature map $\mathbf{X} \in \mathbb{R}^{N \times C}$ of $N$ spatial positions and $C$ channels and outputs a matrix $\mathbf{Z}$ of the same dimensionality

$$
\mathbf{Z} = \mathbf{Y} + \mathbf{X} = f(\mathbf{X})g(\mathbf{X}) + \mathbf{X}
$$

where $f: \mathbb{R}^{N \times C} \rightarrow \mathbb{R}^{N \times N}$ is a pairwise function that calculates the similarity for each pair of spatial positions, and $g: \mathbb{R}^{N \times C} \rightarrow \mathbb{R}^{C \times C}$, is a unary projection function computing a new representation for the input. In the case where $g(\mathbf{X})$ is a linear embedding and $f(\mathbf{X})$ is a dot-product, the formulation of the Non-local block can be defined as

$$
\mathbf{Y}^{NL} = \left( \mathbf{XW}_g \mathbf{W}_g^T \mathbf{X}^T \right) \left( \mathbf{XW}_g \right) = \mathbf{XW}_g \mathbf{X}^T \mathbf{XW}_g,
$$

where $\mathbf{W}_g, \mathbf{W}_g, \mathbf{W}_g$ are learnable parameters of dimension $C \times C$. Formally, the dependencies singled-out by Eq. (7) are clearly highlighted in its element-wise formula as follows:

$$
y_{[a,b]} = \sum_{d,f,h}^{N} C \sum_{e}^{C} w_{f(d,f), g(h,b), e} x_{(a,d)} x_{(e,f)} x_{(e,h)},
$$

where the scalars $w_{f(d,f),g(h,b),e}$ identify the elements of the matrices $\mathbf{W}_f, \mathbf{W}_g$ at given indexes $d, f, h, b$.

Note that the Non-local block in Eq. (7) can be viewed as a special case of $3^{rd}$ order polynomials defined in Eq. (4) and can be alternatively computed using a special tensor of parameters $\mathbf{W}_g^{[NL]}$ block-sparse, low-rank, and decomposed through the matrices $\mathbf{W}_g$ and $\mathbf{W}_f$ matrices. In particular, Eq. (5) coincides with Eq. (8) upon choosing weights $w_{f(d,f), g(h,b), e}$ null for every $c$ different from $a$, $g$ different from $h$, and equal to the Non-local block weights in the remaining cases. The major drawback of this module is its complexity. The Non-local block generates the output $\mathbf{Y}$ by computing the dot-product between a similarity matrix ($\mathbf{XW}_g \mathbf{X}^T$) $\in \mathbb{R}^{N \times N}$ and the embedded input ($\mathbf{XW}_g$) $\in \mathbb{R}^{N \times C}$. This matrix multiplication recalibrates the features at all input positions by aggregating information from all the others.

The pairwise function provides the similarity weights for the contribution of each position and uses a matrix multiplication along the $N$ dimension. The matrix multiplication on the $N$ dimension is at the core of the non-local processing but it introduces a quadratic term in computation that makes the complexity of this module equal to $O(N^2)$.

To address this drawback we propose Poly-NL, a non-local module that does not need any matrix multiplications along the spatial dimension $N$. Analogously to Eq. (6), Poly-NL takes in input a matrix $\mathbf{X} \in \mathbb{R}^{N \times C}$ and outputs a matrix of the same dimensionality $\mathbf{Z}$, that can be computed as

$$
\mathbf{Z} = \alpha \mathbf{X} + \beta \mathbf{Y}^{Poly-NL},
$$

with the additional $\alpha$ and $\beta$ learnable scalars. The matrix $\mathbf{Y}^{Poly-NL}$ is the core of the Poly-NL layer and can be written as follows

$$
\mathbf{Y}^{Poly-NL} = \left( \Psi \left( \mathbf{XW}_1 \circ \mathbf{XW}_2 \circ \mathbf{X} \right) \right) \mathbf{W}_3,
$$

where $\Psi: \mathbb{R}^{N \times C} \rightarrow \mathbb{R}^{N \times C}$ is an average pooling followed by an expansion function on the spatial positions, $\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3 \in \mathbb{R}^{C \times C}$ are matrices of learnable parameters and $\circ$ indicates an element-wise multiplication.

The set of spatial interactions associated with Poly-NL is clearly highlighted in its element-wise formula as follows:

$$
y_{[a,b]}^{Poly-NL} = \sum_{d,f,h}^{N} C \sum_{e}^{C} w_{1(d,f), w_{2(d,b), e}, x_{(a,d)} x_{(e,f)} x_{(e,h)}},
$$

where the values $w_{1(d,f), w_{2(d,b), e}}$ refer to the parameters of the matrix $\mathbf{W}_1 = \mathbf{W}_1 / N$. As visible from the comparison between the two element-wise formulas, Poly-NL and Non-Local block modules are closely connected. In the Non-local block, each element of the output matrix $y_{[a,b]}^{NL}$ is computed using the contribution of a set of triplets $x_{(a,d)} x_{(e,f)} x_{(e,h)}$ weighted using the learnable parameters $w_{1(d,f), w_{2(d,b), e}}$. In Poly-NL, each element of the output matrix is computed using the contribution of the exact same set of triplets, weighted using a different set of learnable parameters. Moreover, Poly-NL is a special case of $3^{rd}$ order polynomials and can be computed as in Eq. (4), upon choosing a $\mathbf{W}_g^{[Poly-NL]}$ block-sparse and decomposed by the matrices $\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3$. Nevertheless, the two modules differ considerably in terms of computational efficiency. Poly-NL does not need to explicitly compute any pairwise-function and can be therefore viewed as a linear complexity alternative to the Non-Local blocks. A diagram of the proposed module is presented in Figure 1.

### 4.2 Poly-SA Layer

In this section, we discuss and extend our polynomial non-local module from a transformer perspective. As introduced in [2] a self-attention block shares the same underlying attention mechanism with the non-local layer but differs in the choice of embedding matrices and the similarity function. The output $\mathbf{Y}$ of a self-attention block is computed as follows:

$$
\mathbf{Y} = \sigma \left( \mathbf{QK}^T / \sqrt{C_q} \right) \mathbf{V},
$$

In particular, a self-attention block takes as input a feature map $\mathbf{X} \in \mathbb{R}^{N \times C}$ of $N$ tokens and $C$ channels. The input is projected into keys $\mathbf{K} = \mathbf{XW}_k$, queries $\mathbf{Q} = \mathbf{XW}_q$ and values $\mathbf{V} = \mathbf{XW}_v$ by the learnable parameters $\mathbf{W}_k \in \mathbb{R}^{C \times C_k}$, $\mathbf{W}_q \in \mathbb{R}^{C \times C_q}$, $\mathbf{W}_v \in \mathbb{R}^{C \times C_v}$. In a standard self-attention
layer, the keys and queries are used to compute an attention matrix and a softmax normalization function $\sigma$ is used to obtain the weights on the values. Analogously to the non-local block, the complexity of Eq. (11) is quadratic with respect to the input size $N$ and the matrix $\sigma \left( QK^T / \sqrt{C_q} \right) \in \mathbb{R}^{N \times N}$ holds the similarity among every possible pair of spatial positions $x_e x_f$ computed with an asymmetric softmax attention kernel. In the remainder of this work, we omit the channel-wise renormalization term $1 / \sqrt{C_q}$ since we can equivalently renormalize input keys and queries. The element-wise form of Eq. (11) reads:

$$y_{a,b} = \sum_{e}^{N} \left( \sum_{d,f,g} \sum_{e,f,g} w_{q(f,g)} x_{a,d} x_{e,f,g} C \sum_{h} X_{e,f} w_{v(h,b)} \right) / C.$$  

(12)

In order to build a formulation that can consider the same set of triplets as the original self-attention, while having linear complexity with respect to both input dimensions, we proceed in two consecutive steps. Firstly, we start by viewing the attention mechanism of Eq. (11) through kernelization. We follow the established literature of [64], [59], [65], [66], [69] and consider a generalized self-attention matrix $\mathbf{Y}_{SA} = \mathbf{A} \mathbf{V} = \left( \phi \left( \mathbf{Q} \right) \phi \left( \mathbf{K} \right)^T \right) \mathbf{V}$, where the softmax attention matrix of the traditional self-attention is replaced with a generic similarity matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$. Specifically, here we consider $\mathbf{A}$ as a linear dot product of the rows in $\mathbf{Q}$ and $\mathbf{K}$ mapped via function $\phi$ designed to generate positive similarity measures. The associative property of matrix multiplications can be used to decrease the complexity of Eq. (13):

$$\mathbf{Y}_{SA} = \left( \phi \left( \mathbf{Q} \right) \phi \left( \mathbf{K} \right)^T \right) \mathbf{V} = \phi \left( \mathbf{Q} \right) \left( \phi \left( \mathbf{K} \right)^T \mathbf{V} \right) = \phi \left( \mathbf{Q} \right) \mathbf{B},$$  

(14)

where the matrix $\mathbf{B} \in \mathbb{R}^{C_q \times C_q}$ characterizes the relationships among channels. This approximation makes the self-attention computation linear with respect to $N$, but also comes with the disadvantage of losing spatial adaptivity. In fact, Eq. (14) replaces a spatial mixing layer with an additional channel mixing block, that can be seen as a dynamic linear layer with weighting matrix $\mathbf{B}$ generated on the fly. This makes the response of all the layers in the ViT identical no matter the spatial position considered. It other words, Eq. (14) has two main characteristics: i) adapts the response of the layer depending on the input $\mathbf{X}$ ii) mixes all channels contribution together. While the first property allows for a switch from static to dynamic neural network [70], the second one is potentially redundant: ViT architectures already deploy a set of linear layers in their MLPs. Therefore, as second step to reduce complexity, we propose to consider only the diagonal of $\mathbf{B}$, that estimates the "importance" of each channel, and use this information to rescale the input:

$$\mathbf{Y}_{Poly-SA} = \phi \left( \mathbf{Q} \right) \text{Diag}(\mathbf{B}).$$  

(15)

This layer maintains the dynamic aspect of Eq. (14), but reduces extra computations. Moreover, Eq. (15) has a direct link with the Poly-NL formulation. Similarly to Eq. (9), can be computed via average-pooling and element-wise multiplications only:

$$\mathbf{Y}_{Poly-SA} = \phi \left( \mathbf{Q} \right) \otimes \Psi \left( \phi \left( \mathbf{K} \right) \otimes \mathbf{V} \right),$$  

(16)

where we consider $\phi$ to be the identity function and therefore the similarity kernel to be a linear kernel. Under this assumption, the element-wise form for Eq. (16) reads:

$$y_{a,b} = \sum_{e}^{N} \sum_{d,f,g} w_{k(d,e)} w_{q(f,g)} x_{e,f} x_{e,f} x_{a,d}.$$  

(17)

From the above equations, it is easy to recognize this formulation as a third-order polynomial block of linear complexity with respect to $N$ and $C$. Furthermore, the dependencies captured by this module closely mimic those considered in the original self-attention: a side-by-side comparison of Eq. (12) and Eq. (17) shows how, for both modules, the output is computed by considering a weighted sum of the $x_{e,f} x_{e,f} x_{a,d}$ interactions of the input. Nevertheless, due to its diagonal form, the block of Eq. (16) scales every spatial position equally and, to be used as an efficient alternative to self-attention in ViT, still lacks a way to re-introduce spatial adaptivity in its formulation without losing its low runtime and memory requirements. We propose to overcome this problem by using two vectors of learnable parameters, $p_1 \in \mathbb{R}^{N}$ and $p_2 \in \mathbb{R}^{N}$, to automatically adjust the attention quantities to each spatial position. Lastly, to avoid convergence problems during training, we wrap the value of the dynamic weights with a sigmoid normalization function.

In conclusion, the equation for Poly-SA reads:

$$\mathbf{Y}_{Poly-SA} = \mathbf{Q} \otimes \begin{bmatrix} 1 & \sigma \left( \mathbf{P} \right) \end{bmatrix}.$$  

(18)

Compared to Poly-NL, Poly-SA maintains the embeddings as proposed in the original self-attention block, it keeps characteristics of spatial adaptivity, and use a $\sigma$ normalization functions to ensure training stability. Therefore, its equation can be naturally extended to the multi-head case described in [2]. Specifically, to create the multi-head extensions, the self-attention formula of Poly-SA is first applied in parallel $h$ times, then the output of each attention head is concatenated along the channel dimension (resulting in feature dimension $hC_k$), and finally the concatenated tensor is projected by $\mathbf{W}_{\text{out}} \in \mathbb{R}^{hC_k \times C}$ to produce the output $\mathbf{Z} = \left[ \mathbf{Y}_0, \ldots, \mathbf{Y}_h \right]$ $\mathbf{W}_{\text{out}} \in \mathbb{R}^{hN \times C}$ having same dimensionality as the input.

5 Experiments

In this section, we demonstrate the ability of our modules to work as a drop-in replacement in existing computer-vision networks, while leaving the exploration of new transformer architectures to future work. Specifically, we showcase the capacity of Poly-NL and Poly-SA to enrich features on established CNN and ViT backbones.

5.1 Poly-NL for CNNs

We evaluate the proposed Poly-NL on three different tasks: object detection and instance segmentation on COCO [71], image classification on ImageNet [72], and face detection
Spatial Positions = 100 x 100

Channels = 1024

Spatial Positions = 100 x 100

Channels = 1024

Max Memory usage [GB]

Table 1: Results of non-local variants for image classification on ImageNet and instance segmentation on COCO. Performance metrics are reported next to FLOPS count (Att-F) and parameters count (Att-P) for each attention module, computed considering an input of size 14 × 14 × 1024 and using the fvcore package.

<table>
<thead>
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<th>Method</th>
<th>Att-F (G)</th>
<th>Att-P (M)</th>
<th>Top-1</th>
<th>Top-5</th>
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<tr>
<td>+ Poly-NL</td>
<td>0.14</td>
<td>0.7</td>
<td>76.30</td>
<td>93.06</td>
</tr>
</tbody>
</table>

(a) ImageNet

<table>
<thead>
<tr>
<th>Method</th>
<th>AP\textsuperscript{b}</th>
<th>AP\textsuperscript{50}</th>
<th>AP\textsuperscript{75}</th>
<th>AP\textsuperscript{m}</th>
<th>AP\textsuperscript{50m}</th>
<th>AP\textsuperscript{75m}</th>
</tr>
</thead>
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<tr>
<td>MaskR-CNN</td>
<td>37.9</td>
<td>59.2</td>
<td>41.0</td>
<td>34.6</td>
<td>56.0</td>
<td>36.9</td>
</tr>
<tr>
<td>+ NL Block</td>
<td>38.8</td>
<td>60.6</td>
<td>42.0</td>
<td>35.4</td>
<td>57.3</td>
<td>37.7</td>
</tr>
<tr>
<td>+ TESA</td>
<td>39.5</td>
<td>60.9</td>
<td>43.1</td>
<td>35.4</td>
<td>57.4</td>
<td>37.5</td>
</tr>
<tr>
<td>+ LatentGNN</td>
<td>38.9</td>
<td>60.4</td>
<td>42.4</td>
<td>35.3</td>
<td>57.3</td>
<td>37.4</td>
</tr>
<tr>
<td>+ EA</td>
<td>38.9</td>
<td>60.3</td>
<td>42.2</td>
<td>35.4</td>
<td>57.2</td>
<td>37.7</td>
</tr>
<tr>
<td>+ Poly-NL</td>
<td>39.2</td>
<td>60.8</td>
<td>42.2</td>
<td>35.4</td>
<td>57.4</td>
<td>37.6</td>
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</tbody>
</table>

(b) COCO

Fig. 2: Runtime and Peak memory consumption performance comparison between Poly-NL and other non-local methods executed on a RTX2080 GPU. Poly-NL exhibits lower computational overhead than competing methods, which is of importance with an increasing number of spatial positions or channels.

5.1.1 Efficiency

We examine the performance of five different layers (TESA [46], NL [3], LatentGNN [63], EA [62] and Poly-NL) to showcase how the proposed solution is able to process inputs with size unmanageable by other formulations. Figure 2 depicts the complexity overhead of various non-local blocks for different sizes of the input matrix X. In the visualization, we examine both the number of spatial positions (Figures 2b and 2c) and the number of channels (as in Figure 2a). We report the runtime on GPU\textsuperscript{1} (Figure 2a, 2b) as a measure of time complexity and the peak memory usage on GPU as indicator of space complexity (Figure 2c). To highlight the impact of computing the non-local interactions, we also include a baseline layer of similar number of parameters (CONV), where no attention mechanism is used. Specifically, we pass the input through the same convolution layers used in a non-local block, but avoid the computation of the attention formula. All benchmarks were executed on single individual block for each method on an identical hardware, under comparable implementations and hyper-parameters. In particular, we highlight the efficiency trends of different long-range interactions computations. In particular, to isolate the contribution of the attention mechanism in the overall computations, we consider for all methods a single block with a single head and a channel reduction factor equal to 1. For each method, the values shown in the charts are the median of 20 runs. Here, the median is used to avoid the effect of potential outliers in the estimate. As can be seen from Figures 2b and 2c, increasing the number of spatial positions greatly impacts efficiency. Runtimes of TESA and NL, which both depend quadratically on the number of spatial positions N, quickly become impractical, even when N is relatively small. Efficient methods (EA, LatentGNN, Poly-NL) scale better with increasing N. Nonetheless, our method holds a competitive advantage in all cases, due to its lack of any matrix dot-product multiplications. As shown in Figure 2a, the number of channels is linearly proportional to the runtime performance of most methods, with the notable exception of TESA. However note that the proposed Poly-NL is considerably faster than the compared methods especially when the number of channels becomes significant. Finally, we highlight how Poly-NL is able to retain access to third order interactions with a complexity on par with the convolutional block (CONV) since by design it extracts the set of non-local interactions by avoiding the explicit computation of any attention matrix.

5.1.2 Classification

We evaluated our method on large-scale image classification, using ImageNet dataset [72], counting 1.28M training images split into 1000 classes. For all the experiments, we modify a ResNet-50 architecture [34] by inserting a non-local module at stage Res4 and then train from scratch with 8 GPUs for 90 epochs, using a batch size of 256 and an SGD optimizer with an initial learning rate of 0.1 and weight decay as described in [74]. We compare our method against four different spatial non-local layers, the original non-local module at stage Res4 and then train from scratch with 8 GPUs for 90 epochs, using a batch size of 256 and an SGD optimizer with an initial learning rate of 0.1 and weight decay as described in [74]. We compare our method against four different spatial non-local layers, the original non-local module at stage Res4 and then train from scratch with 8 GPUs for 90 epochs, using a batch size of 256 and an SGD optimizer with an initial learning rate of 0.1 and weight decay as described in [74].
local block of [3], the efficient LatentGNN variant of [63], the Efficient Attention of [62] and the recently proposed TESA [46]. For the NL block we set the number of channels for the embedding matrices to be half of the input channels. Similarly, for TESA we use a channel reduction factor of 2. For the LatentGNN block we use 2 latent kernels, latent dimension equal 100 and a channel reduction factor of 8. For EA we use a channel reduction factor of 8, a head count of 1 and softmax normalization. For Poly-NL we use a channel reduction factor of 4 by placing the block between a convolutional bottleneck and a convolutional expansion layers. Quantitative results are reported in Table 1a and show the Top-1 and the Top-5 accuracy for the compared methods. Beyond the performance metrics, we also report the number of parameters and FLOPS count for the evaluated methods using the publicly available fvcore package and assuming input of $N = 14$ and $C = 1024$. Poly-NL achieves the best performance on Top-5 accuracy, and on Top-1, outperforms significantly all other non-local neural networks with the exception of TESA [46], which is however computationally very demanding.

5.1.3 Instance Segmentation

We tested our method on object detection and instance segmentation, where the network processes an image and produces a pixel-wise mask that identifies both the category and the instance for each object. We use the Mask R-CNN baseline of [75] trained on MS-COCO 2017 dataset [71], which consists of 118k images as training set, 5k as validation set, and 20k as test set. The Mask R-CNN architecture is composed of a ResNet-FFP backbone for feature extraction followed by a stage that predicts class and box offsets. We used as backbones ResNet-50 [34] architectures pre-trained on ImageNet [72]. We trained with 8 Tesla V-100 GPUs and 2 images per GPU (effective batch size 16) using random horizontal flip as augmentation during training. We use an SGD solver with weight decay of 0.0001, momentum of 0.90, and an initial learning rate of 0.002. All models are trained for 26 epochs with learning rate steps are executed at epoch 16 and 22 with gamma 0.1. In all the experiments, we report the standard metrics of Average Precision $AP$, $AP_{50}$, and $AP_{75}$ for both bounding boxes and segmentation masks.

Following prior work, we modify the Mask R-CNN backbone by adding one non-local layer right before the last residual block of Res4. This procedure highlights the ability of non-local blocks to boost features representation and consequently improve the quality of the candidate object bounding boxes. We compare our method against four different spatial non-local layers, the original non-local block of [3], the efficient LatentGNN variant of [63], the Efficient Attention of [62] and the recently proposed TESA [46]. For a fair comparison, we report the results from our training, achieved using public available source codes and hyper-parameters as provided by the respective authors. Quantitative results are summarized in Table 1b. When compared to the best performing method, TESA [46], Poly-NL exhibits identical performance in $AP_{mask}$ and slightly lower accuracy for $AP_{box}$. However, we note that our proposed method is nearly $10^2$ faster to compute than TESA at the given resolution. Moreover, compared to the non-local layer [3] and its efficient variants LatentGNN [63] and Efficient-Net [62], our method improves performance by 0.3% $\uparrow$ in $AP_{box}$ while keeping linear computational complexity.

5.1.4 2nd and 3rd Order Methods

In this section we briefly discuss the link between our polynomial framework for attention and popular building blocks for neural networks that can be framed as $nd$ order polynomial blocks. We discuss how the use of $nd$ order interactions could boost results on instance segmentation as well as classification but leave a more thorough exploration of this link to future work.

As visible in the element-wise formula of Eq. (3), the use of a block including all possible set of interactions introduces an intractably high amount of parameters and, for this reason, no existing layer can possibly implement such complete formulation. Nevertheless, there are some building blocks which use a low-rank parameter tensor $\mathcal{W}^{[d]}$ decomposed through smaller matrices, and thus can be framed as special cases of this general formula. Specifically, we focus on two blocks closest to our work: Squeeze and Excitation [36] (SE) and the self-attention block proposed Global Context Network [37] (GC). Differently from Poly-NL, which is based on $nd$ order interactions, these blocks process only $2nd$ order interactions. While $2nd$ order methods avoid the quadratic complexity of non-local layers by design, they consider a smaller set of interactions (i.e. $\sum_{c,r} \sum_{d,f} P(c,d)^2 r(c,f)$). To highlight the importance of higher-level interactions, we provide an ablation on instance segmentation on COCO in Table 2a. We followed the protocol described in Section 5.1.3, and modify a ResNet-50 backbone by adding one extra block at stage Res4 and ablate on various possible choices. We consider SE and GC blocks, together with a $2nd$ adaptation of our method (as defined in Eq. (9)) obtained by replacing ($\mathcal{W}_1 \odot \mathcal{X}$) by only $\mathcal{X}_1$ (Ours-$2nd$ ord). This change makes our block close to SE, with the difference in the use of non-linearities and pooling functions. It is evident that in this task, where non-local patterns are crucial, substituting Poly-NL with $2nd$ order methods causes a drop in performance. As visible from Table 2a, our $2nd$ order results are on par with SE, but lower than Poly-NL, thus highlighting the importance of transitioning to $3rd$ order interactions. Further, Poly-NL maintains better performance when compared with GC, which uses the same contribution for every position and thus lose part of the full interaction patterns. In contrast to this method, Poly-NL retains access to every triplet of the original NL providing in return better performance.

Moreover, we showcase how $2nd$ and $3rd$ order interactions can be used jointly to build more discriminative features. A lot of possible choices exists of $2nd$ order blocks, and the best possible combination of $2nd$ and $3rd$ blocks is left to future work. Here, for the sake of simplicity, we choose a formulation $\mathcal{X} \mathcal{W}_p \star \mathcal{X}$ equivalent to ProdPoly block introduced in [76]. We follow the design of the classification experiment of Section 5.1.2 and test the contribution of each layer separately as well as their impact combined together.

2. https://github.com/facebookresearch/fvcore

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As visible from the results in Table 2b, the use of both MLP, Poly-SA is still able to access the same high number of channels. Nonetheless, compared to an \( C < N \) order method (Pi-Nets) improve results on ImageNet.

As apparent in Figure 3a, while XCA and LA outperform other efficient variants by avoiding the need to compute the attention blocks. It also reports performance parameters count of the architecture and FLOPS used to compute the attention. Table 3 reports architecture size, type of the attention block, parameters count of the architecture and FLOPS used to compute the attention blocks. It also reports performance for all the evaluated methods in terms of Top1 accuracy and shows how, without any hyperparameter and macro-design change, Poly-SA is capable of working as a drop-in replacement of traditional blocks in a variety of different cases. As apparent from the table, Poly-SA reduces the complexity without drastically compromising performance in all five architectures. It saves up to 58% of Flops with less than 2% drop in performance, showing consistent results among the evaluated architectures.

### 5.2 Poly-SA for Transformers

In a transformer architecture, MLP-based neural networks are equipped with self-attention blocks, capable of routing information among distant tokens and integrating long-range interactions in their output. In this section, we use the proposed Poly-SA to replace the standard (and more expensive) formulation of self-attention in various transformer architectures. We discuss the differences with respect to standard self-attention in term of efficiency and present its application on two different computer vision tasks.

#### 5.2.1 Efficiency

Next, we discuss the time-complexity of Poly-SA and compare its efficiency with the standard multi-head self-attention SA [2], the efficient variant XCA [60] and LA [59], as these are closely related to our work. As a measure of time-complexity, we report runtime on GPU together with floating-point operations per second, both expressed as a function of input sizes. Similar to the previous section, we define the absolute lower complexity bound in this scenario by reporting the complexity of a linear layer of comparable size (No-SA). In this scenario, XCA, LA and, Poly-SA keep a linear trend with respect to the input size, while a standard SA mechanism scales its complexity quadratically. Nonetheless, as can be seen from Figures 3c and 3b, Poly-SA outperforms other efficient variants by avoiding the need to access elements outside the cross-covariance diagonal and keeps a complexity on par with No-SA, the baseline linear layer where no attention mechanism is used. In addition, we showcase the scalability of our method by analyzing runtime on GPU as a function of the number of channels. As apparent in Figure 3a, while XCA and LA outperform standard SA only for \( C < N \), the performance of Poly-SA is still adjacent to the No-SA lower bound even for a high number of channels. Nonetheless, compared to an MLP, Poly-SA is still able to access the same \( 3^{rd} \) order dependencies as a traditional multi-head self-attention.

#### 5.2.2 Classification

We evaluated our Poly-SA block on a set of different state-of-the-art Vision Transformers. As a setup, we used the large-scale classification task on the ImageNet dataset, consisting of 1.3M training images, 50K validation images, and 1K object classes. We considered two well-known isotropic architectures with no downsampling layers and three hierarchical Vision transformer architectures. Concretely, as isotropic networks, we considered the traditional ViT [50] trained as in [50] (i.e. DeiT) and the XCiT architecture of [60]. As hierarchical networks, we selected two popular 4-stages Transformers, the Swin architecture of [51] and the MetaFormer architecture of [77]. Lastly, we considered the popular 3-stages Transformer of CvT [52]. For every network, we replace all the self-attention (or cross-covariance self-attention) with our Poly-SA block, leaving the remaining architecture unchanged. We used the publicly available code to replicate the original training setup. For CvT, we considered a stride equal to 1 for the Convolutional Projection VK. For DeiT and Swin Transformers, we use a 3x3 depthwise convolution as projection layer to mix heads content together. In the Metaformer architecture SA is used only in the last two stages. To ensure a fair comparison, we also implement Poly-SA only on the last two stages in our variant. We refer to the original papers for the rest of the architectural hyperparameters and training setup details.

Table 3 reports architecture size, type of the attention block, parameters count of the architecture and FLOPS used to compute the attention blocks. It also reports performance for all the evaluated methods in terms of Top1 accuracy and shows how, without any hyperparameter and macro-design change, Poly-SA is capable of working as a drop-in replacement of traditional blocks in a variety of different cases. As apparent from the table, Poly-SA reduces the complexity without drastically compromising performance in all five architectures. It saves up to 58% of Flops with less than 2% drop in performance, showing consistent results among the evaluated architectures. Next, we evaluate the capacity of our method to provide consistent results across datasets and architectural sizes. To do so, we fix an architecture design and evaluate our method on the classification task using both the small scale dataset of CIFAR-100 and the large scale dataset of ImageNet. We select the state-of-the-art architecture XCiT [60] as baseline comparison. This transformer variant builds on top of the CaiT [53] network, and integrates convolution, layer-scale and class-attention modules to the traditional ViT [10]. Moreover, it replaces traditional self-attention with a cross-covariance self-attention, which is closely related to our work. As suggested by the authors, we followed the training setup as in DeiT [50] and trained for 400 epochs with the AdamW optimizer. We refer to the original paper for a detailed de-
The number of channels is: Nano = 128, Tiny = 192, Small = 384, and Medium = 512. The results for CIFAR-100 and ImageNet are reported on Table 4b and Table 4a, respectively. As visible from the results, despite using only the information on the main diagonal, Poly-SA still maintains performances comparable with XCA, and exhibits consistent performance across datasets and network sizes.

6 Discussion
This work is the first to link self-attention layers and polynomial blocks. We have provided a comprehensive theoretical framework for linear complexity attention and extensive empirical evidence that shows how the proposed Poly-NL...
and Poly-SA modules can replace more-complex non-local and self-attention layers. Nevertheless, extensions to our work are still possible. In this section we briefly discuss potential directions, hoping to open a new interesting line of research around this topic.

Firstly, the use of different types of interactions within the self-attention formula is a promising direction. The spatial self-attention blocks only include $N^3 C^3$ triplets which is actually a small subset of all the $N^3 C^3$ possible $3^rd$ order interactions. For example, even for inputs with small size $N = 8^2$, the percentage of utilized triplets would be less than 0.025% of the total. Among these, many might not be very informative, so the question becomes how to efficiently extract the most meaningful interactions from this exponential space. Moreover, our experiments show how the inclusion of interactions of order different than the $3^{rd}$ can lead to performance improvement. This idea could be fully developed by exploring how different orders of interactions interact with each other and whether or not their best configuration is related to the specific task at hand. We also want to use Poly-NL on MindSpore (https://www.mindspore.cn/), which is a new deep learning computing framework. This exploration is left for future work. Second, spatial self-attention only involves one variant of $3^{rd}$ order polynomials. Future work could explore its relations with other instances of the general formula or even investigate strategies to automatically decompose the tensor of parameters $W_{i}^{[3]}$ into tractable and meaningful factorizations. Lastly, at their core, polynomials compute non-linear dependencies through multiplicative interactions. A complete analysis of the relation between non-linear interactions and non-linear activations for deep learning remains an interesting topic to explore.

7 Conclusion

In this work, we cast the non-local block as a $3^{rd}$ order polynomial in the form of multiplicative interactions between spatial locations of the input. Based on this fact, we propose a novel and fast embodiment of non-local layers named Poly-NL which is able to capture long-range dependencies equivalently to NL with a complexity that scales linearly with the size of the input in both computational complexity and memory requirements. Then, we extend our formulation to fit in Transformers literature and propose a multi-head self-attention module named Poly-SA. Poly-NL consistently outperforms other non-local modules on image recognition, instance segmentation, and face detection. Poly-SA achieves an equivalent, if not better, performance than $N^3 C^3$ triplets which is actually a small subset of all the $N^3 C^3$ possible $3^rd$ order interactions.

## References


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