Choose a Transformer: Fourier or Galerkin

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Abstract

In this paper, we apply the self-attention from the state-of-art Transformer in Vaswani et al. [58] the first time to a data-driven operator learning problem related to partial differential equations. We put together an effort to explain the heuristics of, and improve the efficacy of the self-attention by demonstrating that the softmax normalization in the scaled dot-product attention is sufficient but not necessary, and have proved the approximation capacity of a linear variant as a Petrov-Galerkin projection. A new layer normalization scheme is proposed to allow a scaling to propagate through attention layers, which helps the model achieve remarkable accuracy in operator learning tasks with unnormalized data. Finally, we present three operator learning experiments, including the viscid Burgers' equation, an interface Darcy flow, and an inverse interface coefficient identification problem. All experiments validate the improvements of the newly proposed simple attention-based operator learner over their softmax-normalized counterparts.

1 Introduction

Partial differential equations (PDEs) arise from almost every multiphysics and biological systems, from the interaction of atoms to the merge of galaxies, from the formation of cells to the change of climate. Scientists and engineers have been working on approximating the governing PDEs of these physical systems for centuries. The emergence of the computer-aided simulation facilitates a cost-friendly way to study these challenging problems. Traditional methods, such as finite element/difference [12, 14], spectral methods [8], etc, leverage a discrete structure to reduce an infinite dimensional operator map to a finite dimensional approximation problem. Meanwhile in the field practice of many scientific disciplines, substantial measurements for PDE-governed phenomena available on discrete grids enable models like Physics-Informed Neural Network (PINN) [47, 43, 30] to exploit measurements on collocation points to approximate PDE solutions.

Nonetheless for traditional methods or data-driven function learners such as PINN, given a PDE, the focus is to approximate a single instance, for example, solving for an approximated solution for one coefficient with a fixed boundary condition. A slight change to this coefficient invokes a potentially expensive re-training of any data-driven function learners. In contrast, an operator learner aims to learn a map between infinite-dimensional function spaces, which is much more difficult yet rewarding. A well-trained operator learner can evaluate many instances without re-training or collocation points, thus saving valuable resources, and poses itself as a more efficient approach in the long run. PDE-related operator learning is a booming new research direction [42, 39, 38, 45, 59, 60], among which notably the Fourier Neural Operator (FNO) [40] shows an awing state-of-art performance outclassing previous methods by orders of magnitudes in certain benchmarks.

Under a supervised setting, an operator learner is trained with the operator's input functions and their responses to the inputs as targets. Since both functions are sampled at discrete grid points, this is a special case of a `seq2seq` problem [53]. The current state-of-art `seq2seq` model is the Transformer first introduced in [58]. As the heart and soul of the Transformer, the scaled dot-product attention

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mechanism is capable of unearthing the hidden structure of an operator by capturing long-range interactions. Inspired by many insightful pioneering work in Transformers [31, 11, 49, 61, 55, 64, 65, 63, 41, 50, 46], we have modified the attention mechanism by removing the softmax nonlinearity to better serve the purpose of operator learning. A new scale-preserving layer normalization scheme is proposed to enable the attention-based operator learner to better comprehend certain physical properties associated with the PDEs such as the energy decay.

Main contributions. The main contributions of this work are summarized as follows.

- **Attention without softmax.** We propose a new simple scale-preserving self-attention operator and its linear variant without the softmax normalization. Two new interpretations are offered, together with the approximation property of the linear variant proved as a Petrov-Galerkin projection, provided that the feature map can preserve the spacial structures of certain latent representation Hilbert spaces.
- **Operator learner for parametric PDEs.** We combine the newly proposed attention operators with the current best state-of-art operator learner Fourier Neural Operator (FNO) [40] to significantly improve its evaluation accuracy in parametric PDE solution operator learning benchmark problems. Moreover, the new model is capable of recovering coefficients based on noisy measurements that traditional methods or FNO cannot accomplish.
- **Experimental results.** We present three benchmark problems to show that operator learners using the newly proposed attentions are superior in computational/memory efficiency, as well as in accuracy versus those with the conventional softmax normalization. The PyTorch codes to reproduce our results are available as an open-source software. [1]

2 Operator learning involving parametric PDEs

Closely following the setup in [38, 40], we consider a data-driven model to approximate a densely-defined operator $T : \mathcal{H}_1 \to \mathcal{H}_2$ between two Hilbert spaces with an underlying bounded spacial domain $\Omega \subset \mathbb{R}^m$. The operator of interest is usually related to certain physical problems, of which the formulation is to seek the solution to the following parametric PDE for $a \in \mathcal{A}$ where $\mathcal{A}$ stands for the Hilbert space of coefficients:

$$\text{Find } u \in \mathcal{X}, \text{ such that } L_a(u) = f, \quad \text{given } \ f \in \mathcal{Y}. \tag{1}$$

We are interested in the following operator learning problems to approximate T related to (1):

(i) To approximate the nonlinear mapping from the varying parameter a to the solution with a fixed right hand side, $T : \mathcal{A} \to \mathcal{X},\ a \mapsto u$.

(ii) The inverse coefficient identification problem to recover the coefficient from a noisy measurement $\tilde{u}$ of the steady-state solution u, in this case, $T : \mathcal{X} \to \mathcal{A},\ \tilde{u} \mapsto a$.

Using (i) as an example, based on the given N observations $\{a^{(j)}, u^{(j)}\}_{j=1}^N$ and their approximations $\{a_h^{(j)}, u_h^{(j)}\}$ defined at a discrete grid of size $h \ll 1$, the goal of our operator learning problem is to build an approximation T_θ to T, such that $T_\theta(a_h)$ is a good approximation to $u = L_a^{-1} f =: T(a) \approx u_h$ independent of the mesh size h, where a_h and u_h are in finite dimensional spaces $\mathbb{A}_h, \mathbb{X}_h$ on this grid. We further assume that $a^{(j)} \sim \nu$ for a measure ν compactly supported on $\mathcal{A}$, and the sampled data form a reasonably sized subset of $\mathcal{A}$ representative of field applications. The loss $\mathcal{J}(\theta)$ is

$$\mathcal{J}(\theta) := \mathbb{E}_{a\sim\nu}\left[\|\big(T_\theta(a) - u\|_{\mathcal{H}}^2 + \mathfrak{G}(a, u; \theta)\right] \tag{2}$$

and in practice is approximated using the sampled observations on a discrete grid

$$\mathcal{J}(\theta) \approx \frac{1}{N}\sum_{j=1}^{N}\left\{\left\|\big(T_\theta\big(a_h^{(j)}\big) - u_h^{(j)}\right\|_{\mathcal{H}}^2 + \mathfrak{G}\big(a_h^{(j)}, u_h^{(j)}; \theta\big)\right\}. \tag{3}$$

In example (i), $\|\cdot\|_{\mathcal{H}}$ is the standard L^2-norm, and $\mathfrak{G}(a, u; \theta) := \gamma\|a\nabla(T_\theta(a) - u)\|_{L^2(\Omega)}^2$ serves as a regularizer with strength γ and is problem-dependent. In (i) it is added due to knowing the regularity of the target $u \in H^{1+\alpha}(\Omega)$ ($\alpha > 0$ depends on the regularity of a) and $a\nabla u \in \boldsymbol{H}(\mathrm{div}; \Omega)$ a priori. For the evaluation metric, we drop the $\mathfrak{G}(a, u; \theta)$ term, and monitor the minimization of (3) using $\|\cdot\|_{\mathcal{H}}$.

[1] Please download the anonymized codes from the supplemental material.

3 Attention-based operator learner

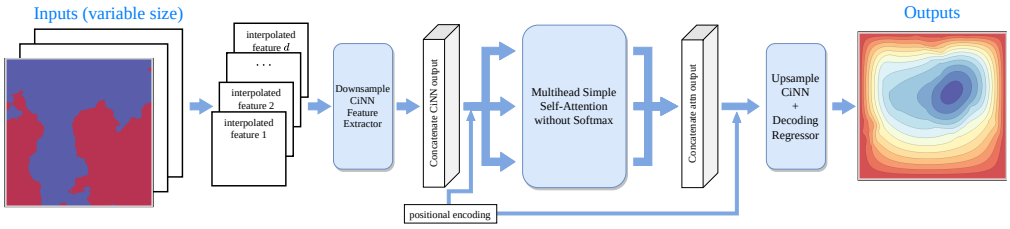

Figure 1: An attention-based operator learner on $\Omega \subset \mathbb{R}^2$.

Feature extractor. We assume the functions in both inputs and targets are sampled on a uniform grid. In an operator learning problem on $\Omega \subset \mathbb{R}^1$, a simple feedforward neural network (FFN) is used as the feature extractor that is shared by every position (grid point).

Interpolation-based CNN. If $\Omega \subset \mathbb{R}^2$, inspired by the Vision Transformer (ViT) [17] and the multilevel graph kernel network in [38], we use two 3-level interpolation-based CNNs (CiNN) as the feature extractor, but also as the downsampling and upsampling layer, respectively, in which we refer to restrictions/prolongations between the coarse/fine grids both as interpolations. See Figure 1.

Positional encoding. We simply concatenate the Cartesian coordinates of each grid point as additional feature dimension(s) to the input data, as well as to the latent representations in every attention head. In 2D problems, there are fine and coarse grids, and only the coarse grid positional encoding of size $n_c \times n_c \times 2$ is concatenated to the latent representations before flattening. As a result, the input/output dimensions of an attention-based encoder layer are both $n_c^2 \times d$. Nevertheless inside an encoder layer, the propagation runs for a tensor of size $n_c^2 \times (d + m \cdot (\texttt{nhead}))$.

Decoder. The decoder is a problem-dependent admissible network that maps the learned representations from the encoder back to the target dimension. For smooth and regular solutions in $H^{1+\alpha}(\Omega)$, we opt for a 2-layer spectral convolution that is the core component in [40]. A simple pointwise feedforward neural network (FFN) is used for nonsmooth targets in $L^\infty(\Omega)$.

3.1 Simple self-attention encoder

The encoder contains a stack of identical simple attention-based encoder layers. For simplicity consider a single attention head that maps $\mathbf{y} \in \mathbb{R}^{n \times d}$ to another element in $\mathbb{R}^{n \times d}$, define the trainable projection matrices, and query, keys, values as follows.

$$W^Q, W^K, W^V \in \mathbb{R}^{d \times d}, \quad \text{and} \quad Q := \mathbf{y}W^Q, \quad K := \mathbf{y}W^K, \quad V := \mathbf{y}W^V. \tag{4}$$

We propose the following simple attention that (i) uses a mesh-weighted normalization without softmax, (ii) allows a scaling to propagate through the encoder layers.

$$\mathrm{Attn}_{\mathrm{sp}} : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d}, \quad \mathbf{y} \mapsto \mathbf{y} + \sigma\big(\mathbf{y} + \mathrm{Attn}_\dagger(\mathbf{y})\big), \tag{5}$$

where the head-wise normalizations are applied pre-dot product: for $\dagger \in \{\mathfrak{f}, \mathfrak{g}\}$,

$$\text{(Fourier-type local attention)} \qquad \mathbf{z} = \mathrm{Attn}_\mathfrak{f}(\mathbf{y}) := (\widetilde{Q}\widetilde{K}^\top)V/n, \tag{6}$$

$$\text{(Galerkin-type global attention)} \qquad \mathbf{z} = \mathrm{Attn}_\mathfrak{g}(\mathbf{y}) := Q(\widetilde{K}^\top\widetilde{V})/n, \tag{7}$$

and $\widetilde{\diamond}$ denotes a trainable non-batch-based normalization. As in the classic Transformer [58], we choose $\widetilde{\diamond}$ as the layer normalization $\mathrm{Ln}(\diamond)$, and $\sigma(\cdot)$ as the standard 2-layer FFN identically applied on every position (grid point). In simple attentions, the weight of each position of values, or that of query in the linear variant, is not all positive anymore. This can be viewed as a cheap alternative to the cosine similarity-based attention.

Remark 3.1. *If we apply the regular layer normalization rule that eliminates any scaling:*

$$\mathbf{y} \mapsto \mathrm{Ln}\big(\mathbf{y} + \sigma\big(\mathrm{Ln}(\mathbf{y} + \mathrm{Attn}_\dagger(\mathbf{y}))\big)\big), \quad \textit{where} \ \mathrm{Attn}_\dagger(\mathbf{y}) := (QK^\top)V/n = Q(K^\top V)/n, \tag{8}$$

then this reduces to the efficient attention first proposed in [50].

3.1.1 Spacial structure-preserving feature map

Consider an operator learning problem with an underlying domain $\Omega \subset \mathbb{R}^1$. $\{x_l\}_{l=1}^n$ denotes the set of grid points in the discretized Ω such that the weight $1/n = h$ is the mesh size. Let $\zeta_q(\cdot), \phi_k(\cdot), \psi_v(\cdot) : \Omega \to \mathbb{R}^{1\times d}$ denote the feature maps of Q, K, V, i.e., the i-th row of Q, K, V written as $\boldsymbol{q}_i = \zeta_q(x_i)$, $\boldsymbol{k}_i = \phi_k(x_i)$, $\boldsymbol{v}_i = \psi_v(x_i)$. They are, in the NLP convention, viewed as the feature (embedding) vector at the i-th position, respectively. The inter-position topological structure such as continuity/differentiability in the same feature dimension is learned thus not explicit. The following ansatz for Q, K, V in the same attention head is fundamental to our new interpretations.

Assumption 3.2. *The columns of $Q/K/V$, respectively, contain the vector representations of the learned basis functions spanning certain subspaces of the latent representation Hilbert spaces.*

Using $V \in \mathbb{R}^{n\times d}$ with a full column rank as an example, its columns contain potentially a set of bases $\{v_j(\cdot)\}_{j=1}^d$ evaluated at the grid points (degrees of freedom, or DoFs). Similarly, the learned bases whose DoFs form the columns of Q, K are denoted as $\{q_j(\cdot)\}_{j=1}^d$, $\{k_j(\cdot)\}_{j=1}^d$, as well as $\{z_j(\cdot)\}_{j=1}^d$ for the outputs in (6) and (7). To be specific, the j-th column of V, denoted by $\boldsymbol{v}^j$, then stands for a vector representation of the j-th basis function evaluated at each grid point, i.e., its l-th position stands for $(\boldsymbol{v}^j)_l = v_j(x_l)$. Consequently, the row $\boldsymbol{v}_i = (v_1(x_i), \ldots, v_d(x_i))$ can be alternatively viewed as the evaluation of different latent basis functions at x_i.

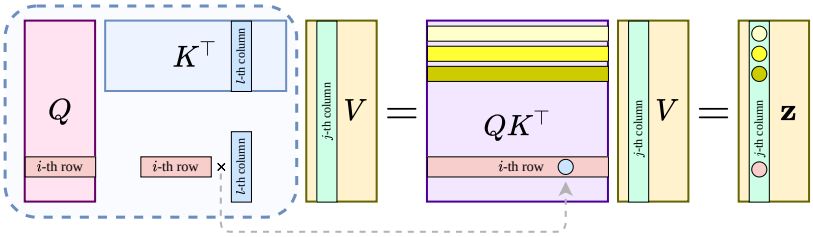

Figure 2: A dissection of Fourier-type attention's output.

3.1.2 Fourier-type attention

In the Fourier-type attention (6), Q, K are assumed to be normalized for simplicity, the j-th column ($1 \le j \le d$) in the i-th row ($1 \le i \le n$) of $\mathbf{z}$ is computed by (see Figure 2):

$$\begin{aligned}(\boldsymbol{z}_i)_j &= h(QK^\top)_{i\bullet}\, \boldsymbol{v}^j = h\big(\boldsymbol{q}_i \cdot \boldsymbol{k}_1, \ldots, \boldsymbol{q}_i \cdot \boldsymbol{k}_l, \ldots, \boldsymbol{q}_i \cdot \boldsymbol{k}_n\big)^\top \cdot \boldsymbol{v}^j \\ &= h \sum_{l=1}^n (\boldsymbol{q}_i \cdot \boldsymbol{k}_l)(\boldsymbol{v}^j)_l \approx \int_\Omega \big(\zeta_q(x_i) \cdot \phi_k(\xi)\big) v_j(\xi)\, \mathrm{d}\xi,\end{aligned} \tag{9}$$

where the h-weight facilitates the numerical quadrature interpretation of the inner product. Concatenating columns $1 \le j \le d$ yields the i-row $\boldsymbol{z}_i$ of the output $\mathbf{z}$:

$$\boldsymbol{z}_i \approx \int_\Omega \big(\zeta_q(x_i) \cdot \phi_k(\xi)\big) \psi_v(\xi)\, \mathrm{d}\xi. \tag{10}$$

Therefore, without the softmax nonlinearity, the local dot-product attention output at i-th row computes approximately an integral transform with a non-symmetric learnable kernel function $\kappa(x, \xi) := \zeta_q(x)\phi_k(\xi)$ evaluated at x_i, whose approximation property has been studied in [63, Theorem 2], yet without the logits technicality due to the removal of the softmax normalization.

After the skip-connection, if we further exploit the learnable nature of the method and assume $W^V = \mathrm{diag}\{\delta_1, \cdots, \delta_d\}$ such that $\delta_j \neq 0$ for $1 \le j \le d$, under Assumption 3.2:

$$\delta_j^{-1} v_j(x) \approx z_j(x) - \int_\Omega \kappa(x, \xi) v_j(\xi)\, \mathrm{d}\xi, \quad \text{for } j = 1, \cdots, d, \quad \text{and } x \in \{x_i\}_{i=1}^n. \tag{11}$$

This is the forward propagation of the Fredholm equation of the second-kind for each $v_j(\cdot)$. When using an explicit orthogonal expansion such as Fourier to solve for $\{v_j\}_{j=1}^d$, or seeking for a better set of $\{v_j\}$ in our case, it is long known that this is equivalent to the Nyström's method with a simple

numerical integration [5] (similar to the $h = 1/n$ weighted sum). Therefore, the successes of the random Fourier features in Performer [11] and the Nyströmformer's approximation [65] are not surprising.

Finally, we name this type of simple attention "Fourier" is due to the striking resemblance between the local scaled dot-product operation and a Fourier-type kernel [20] integral transform, since eventually the target resides in a Hilbert space with an underlying spacial domain Ω, while the latent representation space parallels a "frequency" domain on Ω^*.

3.1.3 Galerkin-type attention

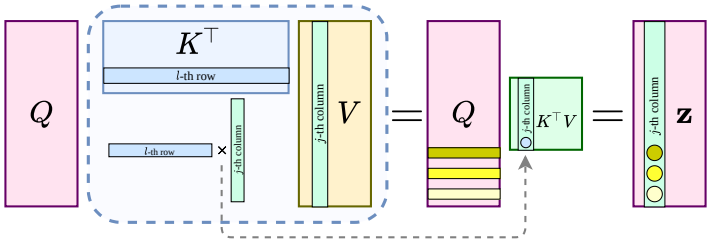

Figure 3: A dissection of Galerkin-type attention's output.

For the Galerkin-type simple attention in (7), K, V are assumed to be normalized for simplicity, we first consider the i-th entry in the j-th column $\boldsymbol{z}^j$ of $\mathbf{z}$ (see Figure 3):

$$(\boldsymbol{z}^j)_i = h\, \boldsymbol{q}_i^\top \cdot (K^\top V)_{\bullet j}, \tag{12}$$

which is the inner product of the i-th row of Q and the j-th column of $K^\top V$. Thus,

$$\boldsymbol{z}^j = h \begin{pmatrix} | & | & | & | \\ \boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_n \\ | & | & | & | \end{pmatrix}^\top (K^\top V)_{\bullet j} = h \left((K^\top V)_{\bullet j}^\top \begin{pmatrix} — & \boldsymbol{q}^1 & — \\ — & \vdots & — \\ — & \boldsymbol{q}^d & — \end{pmatrix} \right)^\top \tag{13}$$

This reads as: $(K^\top V)_{\bullet j}$ contains the coefficients for the linear combination of the vector representations $\{\boldsymbol{q}^l\}_{l=1}^d$ for bases stored in Q's column space to form the output $\mathbf{z}$. Meanwhile, the j-th column of $K^\top V$ consists the inner product of j-th column of V with every column of K.

$$\boldsymbol{z}^j = h \sum_{l=1}^d \boldsymbol{q}^l (K^\top V)_{lj}, \quad \text{where} \;\; (K^\top V)_{\bullet j} = \left(\boldsymbol{k}^1 \cdot \boldsymbol{v}^j, \boldsymbol{k}^2 \cdot \boldsymbol{v}^j, \cdots, \boldsymbol{k}^d \cdot \boldsymbol{v}^j\right)^\top. \tag{14}$$

As a result, using Assumption 3.2's interpretation, i.e., $k_l(\cdot)$, $v_j(\cdot)$ evaluated at every x_i are simply their vector representations $\boldsymbol{k}^l$ ($1 \le l \le d$) and $\boldsymbol{v}^j$, we have the functions represented by the columns of the output $\mathbf{z}$ can be then compactly written as:

$$z_j(x) := \sum_{l=1}^d \mathfrak{b}\big(k_l, v_j\big)\, q_l(x), \quad \text{for } j = 1, \cdots, d, \quad \text{and } x \in \{x_i\}_{i=1}^n, \tag{15}$$

where the bilinear form $\mathfrak{b}(\cdot,\cdot) : \mathcal{K} \times \mathcal{V} \to \mathbb{R}$. If for simplicity the latent Hilbert spaces $\mathcal{K}$ and $\mathcal{V}$ are assumed to be defined on the same spacial domain Ω, (15) can be written in a componentwise form:

$$(\boldsymbol{z}^j)_i = z_j(x_i) = h \sum_{l=1}^d (\boldsymbol{k}^l \cdot \boldsymbol{v}^j)(\boldsymbol{q}^l)_i \approx \sum_{l=1}^d \left(\int_\Omega k_l(\xi) v_j(\xi)\, \mathrm{d}\xi \right) q_l(x_i). \tag{16}$$

Therefore, when $\{\diamond_j(\cdot)\}_{j=1}^d$, $\diamond \in \{q, k, v\}$ consist approximations to three sets of bases for certain potentially different subspaces, and if we set the trial spaces as the column spaces of Q and the test space as that of K, respectively, the forward propagation rule of Galerkin-type attention is a recast of a learnable Petrov–Galerkin-type projection [9, 19] for every basis represented by the columns of V. Essentially, this is a change of basis: how to linearly combine the bases in Q is based on the inner product (response) of the corresponding feature dimension's basis in V against every basis in K. While the form of (16) suggests the orthonormality of the basis represented by Q, K, V, as well as being of full column ranks, the learnable nature of the method suggests otherwise. At last, we have the following strikingly simple yet extremely powerful approximation result.

Theorem 3.3 (Céa-type lemma)**.** *Consider an $f \in \mathcal{H}$, defined on a bounded domain $\Omega \subset \mathbb{R}^m$ discretized by n grid points. $\mathbf{y} \in \mathbb{R}^{n\times d}$ is the current latent representation for $n > d > m$ and full column rank. $\mathbb{Q}_h$ and $\mathbb{V}_h$ are the latent approximation subspaces spanned by basis functions with the columns of Q and V in (4) as degrees of freedom, respectively, and $\dim \mathbb{Q}_h = r \le \dim \mathbb{V}_h = d$. Let $\mathfrak{b}(\cdot,\cdot) : \mathbb{Q}_h \times \mathbb{V}_h \to \mathbb{R}$ be a continuous bilinear form; $g_\theta(\cdot)$ is a learnable map that is the composition of the Galerkin-type attention operator with a new set of attention matrices, and a pointwise universal approximator. If for any fixed $q \in \mathbb{Q}_h$ the functional norm of $\mathfrak{b}(q,\cdot)$ is bounded below by $c > 0$, then it holds for $f_h \in \mathbb{Q}_h$ being the best approximation of f in $\|\cdot\|_{\mathcal{H}}$:*

$$\min_\theta \|f - g_\theta(\mathbf{y})\|_{\mathcal{H}} \le c^{-1} \min_{q\in\mathbb{Q}_h} \max_{v\in\mathbb{V}_h} \frac{|\mathfrak{b}(f_h - q, v)|}{\|v\|_{\mathcal{H}}} + \|f - f_h\|_{\mathcal{H}}. \tag{17}$$

Remarks and interpretations of the best approximation result. Theorem 3.3 states that the Galerkin-type attention has capacity to give a quasi-optimal approximation in $\|\cdot\|_{\mathcal{H}}$ in the current subspace $\mathbb{Q}_h$. For the mathematically rigorous complete set of notations and the full details of the proof we refer the readers to Appendix D. Even though Theorem 3.3 is presented for a single instance of $f \in \mathcal{H}$ for simplicity, the proof in Appendix D shows that the attention operator is fully capable of simultaneously approximating a collection of functions. Estimate (17) comes with great scalability with respect to the sequence length in that it all boils down to whether c is independent of n in the lower bound of $\|\mathfrak{b}(q,\cdot)\|_{\mathbb{V}_h'}$. The existence of an n-independent lower bound is commonly known as the discrete version of the Ladyzhenskaya–Babuška–Brezzi (LBB) condition [13, Chapter 6.12], also referred as the Banach-Nečas-Babuška (BNB) condition in Galerkin methods on Banach spaces [19, Theorem 2.6]. As the cornerstone of the approximation to many PDEs, it establishes the surjectivity of a map from $\mathbb{V}_h$ to $\mathbb{Q}_h$. In the context of the linear variant of the attention operator (Q: values, K: query, V: keys), it roughly translates to: for the best approximator in values, there exists at least one key to match an incoming query to deliver this best approximator.

The role of feed-forward networks. Due to the presence of the concatenated coordinates $\mathbf{x} := \|_{i=1}^n x_i \in \mathbb{R}^{n\times m}$ to the latent representation $\mathbf{y}$, the pointwise subnetwork $\sigma_s(\cdot) : \mathbb{R}^{n\times m} \to \mathbb{R}^{n\times d}$ of the nonlinear universal approximator (FFN) in each attention block is one among many magics of the attention mechanism, in that the subspaces $\mathbb{Q}_h$ and $\mathbb{V}_h$ will be constantly enriched by $\mathrm{span}\{w_j \in \mathbb{X}_h : w_j(x_i) = (\sigma_s(\mathbf{x}))_{ij}, 1 \le j \le d\} \subset \mathcal{H}$ to try to capture how an operator of interest responses to the subset of inputs. Despite the fact that the FFNs, when being viewed as a class of functions, bear no linear structure within, the basis functions produced this way act as a building block to characterize a linear space for a learnable projection.

4 Experiments

In this section we perform a numerical study the proposed Fourier Transformer (**FT**) with the Fourier-type encoder, and the Galerkin Transformer (**GT**) with the Galerkin-type encoder, in various PDE-related operator learning tasks. The models we compare our newly proposed models with are the operator learners with the simple attention replaced by the standard softmax normalized scaled dot-product attention (**ST**) [58], and a linear variant (**LT**) [50] in which two independent softmax normalizations are applied on Q, K separately.[2] The data are obtained courtesy of the PDE benchmark under the MIT license.[3] For full details of the training/evaluation and model structures please refer to Appendix C.

Instead of the standard Xavier uniform initialization [23], for the projection matrices W^Q, W^K, W^V, we modified the initialization slightly as follows

$$W^\diamond_{\text{init}} \leftarrow \eta U + \delta I, \quad \text{for } \diamond \in \{Q, K, V\}, \tag{18}$$

where $U = (x_{ij})$ is a random matrix using the Xavier initialization with gain 1 such that $x_{ij} \sim \mathcal{U}([-\sqrt{3/d}, \sqrt{3/d}])$, and δ is a small positive number. In certain operator learning tasks, we found that this tiny modification boosts the evaluation performance of models by up to 50% (see Appendix C.2) and improves the training stability acting as a cheap remedy to the lack of a softmax normalization.

[2] https://github.com/lucidrains/linear-attention-transformer

[3] https://github.com/zongyi-li/fourier_neural_operator

Unsurprisingly, when compared the memory usage and the speed of the networks (see Table 1), the Fourier-type attention features a 40%–50% reduction in memory versus the attention with a softmax normalization. The Galerkin attention-based models have a similar memory profile with the standard linear attention, it offers up to a 120% speed boost over the linear attention in certain tests.

The baseline models for each example are the best operator learner to-date, the state-of-art Fourier Neural Operator (FNO) in [40] but without the original built-in batch normalization. All attention-based models match the parameter quota of the baseline, and are trained using the loss in (3) with the same `1cycle` scheduler [51] for 100 epochs. For fairness, we have also included the results for the standard softmax normalized models (ST and LT) using the new layer normalization scheme in (6) and (7). We have retrained the baseline with the same `1cycle` scheduler using the code provided in [40], and listed the original baseline results using a step scheduler of 500 epochs of training from [40] Example 5.1 and Example 5.2, respectively.

Table 1: The memory usage and speed comparison of the models. b: batch size; the CUDA mem (GB) is the sum of the `self_cuda_memory_usage` from the PyTorch `autograd` profiler for 1 backpropagation; the mem (GB) is recorded from `nvidia-smi` of the memory allocated for the active Python process during profiling; the speed (iteration per second) is measured during training.

	Example 1: $n = 8192$ ($b = 4$)			Example 2: $n_f = 211$ ($b = 4$)			Encoders only: $n = 8192, d = 128$		
	Mem	CUDA Mem	Speed	Mem	CUDA Mem	Speed	Mem	CUDA Mem	Speed
ST	18.39	31.06	5.02	22.14	40.78	3.95	18.53	31.34	4.12
FT	10.05	22.92	6.10	11.34	30.85	4.55	10.80	22.32	5.46
LT	2.55	2.31	12.70	3.69	5.08	11.40	2.73	2.66	10.98
GT	2.36	1.93	27.15	3.55	4.82	12.03	2.53	2.33	19.20

4.1 Example 1: viscous Burgers' equation

In this example, we consider a benchmark problem of the viscous Burgers' equation with a periodic boundary condition on $\Omega := (0, 1)$ in [40]. The nonlinear operator to be learned is the discrete approximations to the solution operator $T : C_p^0(\Omega) \cap L^2(\Omega) \to C_p^0(\Omega) \cap H^1(\Omega)$, $u_0(\cdot) \mapsto u(\cdot, 1)$. The initial condition $u_0(\cdot)$'s are sampled following a Gaussian Random Field (GRF).

The result can be found in Table 2. All attention-based operator learners achieve a resolution-invariant performance similar with FNO1d in [40]. The new scale-preserving layer normalization scheme significantly outperforms the regular layer normalization rule in this example, in which both inputs and targets are unnormalized. For full details please refer to Appendix C.2.

Table 2: Evaluation relative error ($\times 10^{-3}$) of Burgers' equation 4.1.

	$n = 512$ ($b = 8$)	$n = 2048$ ($b = 8$)	$n = 8192$ ($b = 4$)
FNO1d [40]	15.8	14.6	13.9
FNO1d `1cycle`	4.373	4.126	4.151
FT regular Ln	1.400	1.477	1.172
GT regular Ln	2.181	1.512	2.747
ST regular Ln	1.927	2.307	1.981
LT regular Ln	1.813	1.770	1.617
FT Ln on Q, K	**1.135**	**1.123**	**1.071**
GT Ln on K, V	**1.203**	**1.150**	**1.025**
ST Ln on Q, K	1.271	1.266	1.330
LT Ln on K, V	1.139	1.149	1.221

4.2 Example 2: Darcy flow

In this example, we consider another well-known benchmark $-\nabla \cdot (a\nabla u) = f$ for $u \in H_0^1(\Omega)$ from [7, 40, 38, 45], and the operator to be learned is the approximations to $T : L^\infty(\Omega) \to H_0^1(\Omega), a \mapsto u$, in which a is the coefficient with a random interface geometry, and u is the weak solution.

The result can be found in Table 3. As the input/output are normalized, in contrast to Example 4.1, the scale-preserving propagation scheme does not significantly outperform the regular layer

normalization rule in this example. The attention-based operator learners achieve on average 30% to 50% better evaluation results than the baseline FNO2d using the same trainer. For full details please refer to Appendix C.3.

Table 3: Evaluation relative error ($\times 10^{-2}$) of Darcy interface problem 4.2.

	$n_f = 141, n_c = 43$	$n_f = 211, n_c = 61$
FNO2d [40]	1.09	1.09
FNO2d `1cycle` (only n_f)	1.419	1.424
FT regular Ln	**0.838**	**0.847**
GT regular Ln	0.894	**0.856**
ST regular Ln	1.075	1.131
LT regular Ln	1.024	1.130
FT Ln on Q, K	0.919	0.935
GT Ln on K, V	**0.839**	0.900
ST Ln on Q, K	0.946	0.959
LT Ln on K, V	0.875	0.970

4.3 Example 3: inverse coefficient identification for Darcy flow

In this example, we consider an inverse coefficient identification problem based on the same data used in Example 4.2. The input (solution) and the target (coefficient) are reversed from Example 4.2, and the noises are added to the input. The inverse problems in practice are a class of important tasks in many scientific disciplines such geological sciences and medical imaging but much more difficult due to poor stability [33]. We aim to learn an approximation to an ill-posed operator $T : H_0^1(\Omega) \to L^\infty(\Omega), u + \epsilon N_\nu(u) \mapsto a$, where $N_\nu(u)$ stands for noises related to the sampling distribution and the data. $\epsilon = 0.01$ means 1% of noise added in both training and evaluation, etc.

The result can be found in Table 4. It is not surprising that FNO2d, an excellent smoother which filters higher modes in the frequency domain, struggles in this example to recover targets consisting of high-frequency traits (irregular interfaces) from low-frequency prevailing data (smooth solution due to ellipticity). We note that, the current state-of-art methods [10] for inverse interface coefficient identification need to carry numerous iterations to recover a single instance of a simple coefficient with a regular interface, provided that a satisfactory denoising has done beforehand. The attention-based operator learner has capacity to unearth structurally how this inverse operator's responses on a subset, with various benefits articulated in [38, 40, 39, 45, 7].

Table 4: Evaluation relative error ($\times 10^{-2}$) of the inverse problem 4.3.

	$n_f = 141, n_c = 36$			$n_f = 211, n_c = 71$		
	$\epsilon = 0$	$\epsilon = 0.01$	$\epsilon = 0.1$	$\epsilon = 0$	$\epsilon = 0.01$	$\epsilon = 0.1$
FNO2d (only n_f)	13.71	13.78	15.12	13.93	13.96	15.04
FNO2d (only n_c)	14.17	14.31	17.30	13.60	13.69	16.04
FT regular Ln	**1.779**	**2.467**	6.814	1.563	2.704	8.110
GT regular Ln	2.026	2.536	**6.659**	1.732	2.775	8.024
ST regular Ln	2.434	3.106	7.431	2.069	3.365	8.918
LT regular Ln	2.254	3.194	9.056	2.063	3.544	9.874
FT Ln on Q, K	1.921	2.717	6.936	**1.534**	**2.691**	8.286
GT Ln on K, V	2.149	2.758	6.689	1.799	2.764	**7.903**
ST Ln on Q, K	2.160	2.807	6.995	1.889	3.123	8.788
LT Ln on K, V	2.360	3.196	8.656	2.136	3.539	9.622

4.4 Related Works

Operator learners. In [3, 39], certain kernel forms of the solution operator of parametric PDEs are approximated using graph neural networks. [38] further improves the kernel approach by exploiting the multilevel grid structure. The first discretization-invariant encoder–decoder operator learner is proposed in [40] to achieve a state-of-art performance in certain benchmark problems. [59, 60] first proposed a network equivalent to an additive attention, similar to the one in the Neural Turing

Machine (NMT) in [4]. Other notable approaches to approximate the solution operators of PDEs include [7, 42, 45]. Pure deep convolutional neural network (DCNN)-based operator learners are widely applied to learn the maps with a fixed discretization size, including both the solution operator and the inverse operator with noisy measurements [1, 6, 27, 25, 24, 66, 57]. To our best knowledge, there is no work on data-driven approaches to an inverse interface coefficient identification for a class of coefficients with random interface geometries.

Attention mechanism. Aside from the ground-breaking scaled dot-product attention in [58], earlier [4] proposed an additive content-based attention, however, with a vanishing gradient problem due to multiple nonlinearity composition. [15] shows the first effort in removing the softmax normalization in [4] after the projection, however, it still uses a Sigmoid nonlinearity before the additive interpolation propagation stage, and performs worse than its softmax counterpart. There are various linearization efforts of the scaled dot-product attention operator, notably in [31, 11, 49, 61, 50]. All linear variants of the Transformer leverage the existence of a feature map to formulate the similarity function to form a more general kernel. The conjecture in [49] inspires us to remove the softmax overall. [50] first proposed the $1/n$-scaling normalization for a linear complexity attention without the softmax, however, the scaling normalization has not been extensively studied in examples and performs worse.

Various studies on Transformers. The kernel interpretation in [55] inspires us to reformulate the attention using the Galerkin-projection. Theorem 2 in [63] gives a theoretical foundation of removing the softmax normalization to formulate the Fourier-type attention. The Nyström approximation [65] essentially acknowledges the similarity between the attention matrix and an integral kernel. The experiments of various initializations in [41] inspires us to propose the diagonal dominant initialization scheme used in this paper. [64, 46] inspires us to try different layer normalization schemes. [29, 21, 54] propose attention mechanisms that conserve certain physical properties.

5 Conclusion

We propose a general operator learner based on a simple attention mechanism. The network is versatile and is able to approximate both the PDE solution operator and the inverse coefficient identification operator. The evaluation accuracy on the benchmark problems surpasses the current best state-of-art operator learner Fourier Neural Operator (FNO) in [40]. However, we acknowledge the limitation of this work: (i) similar to other operator learners, the subspace, on which we aim to learn the operator's responses, may be infinite dimensional, but the operator must exhibit certain low-dimensional attributes (e.g., smoothing property of the higher frequencies in GRF); (ii) it is not efficient for the attention operator to be applied at the full resolution for a 2D problem, and this limits the approximation to a nonsmooth subset such as functions in L^∞.

6 Broader Impact

Our work introduces the state-of-art self-attention mechanism the first time to PDE-related operator learning problems. The new interpretations of attentions invite numerical analysts to work on a more complete and delicate approximation theory of the attention mechanism. We have proved the Galerkin-type attention's approximation capacity in an ideal Hilbertian setting. Numerically, the new attention-based operator learner has capacity to approximate the difficult inverse coefficient identification problem with an extremely noisy measurements, which was not attainable using traditional iterative methods for nonlinear mappings. Thus, our method may pose a huge positive impact in geoscience, medical imaging, etc. Moreover, traditionally the embeddings in Transformer-based NLP models map the words to a high dimensional space, but the topological structure in the same feature dimension between different positions are learned thereby not efficient. Our proof provides a theoretical guide for the search of feature maps that preserve, or even create, structures such as differentiability or physical invariance. Thus, it may contribute to the removal of the softmax nonlinearity to speed up significantly the arduous training or pre-training of larger models such as BERT [16], ALBERT [35], etc. However, we do acknowledge that our research may negatively impact on the effort of building a cleaner future for our planet, as inverse problems are widely studied in reservoir detection, and we have demonstrated that the attention-based operator learner could potentially help to discover new fossil fuel reservoirs due to its capacity to infer the coefficients from noisy measurements.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] In Section 5 and in each experiment's detailed description in Appendix C.3 and C.4.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] In Section 6.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] The key assumption of the new interpretations of the attention mechanism is in Assumption 3.2. Due to the page limit, the assumptions and settings are fully elaborated in a mathematical rigorous fashion in Appendix D for the proof of Theorem 3.3.
   (b) Did you include complete proofs of all theoretical results? [Yes] In Appendix D.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] The Python codes are attached in the supplemental material, the data are publicly available. Please refer to `README.md` in the supplemental zip file.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] We include all details in the supplemental material Appendix B and C.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] We found that our method is almost seed-invariant, and we have reported the error bands in Appendix C.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] Please refer to Appendix C.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] Multiple creators of or contributing work to the dataset used in our work are cited [40, 39, 38, 45]. The code base we have implemented our model upon is in the footnote of Section 4, and cited in the Acknowledgement [34]. In the publicly available code repository, in the document of every function, we have credited every author we can find for even a small code snippet, if that function is not built from ground up by us.
   (b) Did you mention the license of the assets? [Yes] In Section 4.
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] The full code base to replicate our results is included in the supplemental material.
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes] The data is obtained from `https://github.com/zongyi-li/fourier_neural_operator` with the MIT license as well as the consent from the author per a personal communication.
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]