ENERGY TRANSFORMER

Anonymous authors
Paper under double-blind review

ABSTRACT

Transformers have become the de facto models of choice in machine learning, typically leading to impressive performance on many applications. At the same time, the architectural development in the transformer world is mostly driven by empirical findings, and the theoretical understanding of their architectural building blocks is rather limited. In contrast, Dense Associative Memory models or Modern Hopfield Networks have a well-established theoretical foundation, but have not yet demonstrated truly impressive practical results. We propose a transformer architecture that replaces the sequence of feedforward transformer blocks with a single large Associative Memory model. Our novel architecture, called Energy Transformer (or ET for short), has many of the familiar architectural primitives that are often used in the current generation of transformers. However, it is not identical to the existing architectures. The sequence of transformer layers in ET is purposely designed to minimize a specifically engineered energy function, which is responsible for representing the relationships between the tokens. As a consequence of this computational principle, the attention in ET is different from the conventional attention mechanism. In this work, we introduce the theoretical foundations of ET, explore it's empirical capabilities using the image completion task, and obtain strong quantitative results on the graph anomaly detection task.

1 INTRODUCTION

Transformers have become pervasive models in various domains of machine learning, including language, vision, and audio processing. Every transformer block uses four fundamental operations: attention, feed-forward multi-layer perceptron (MLP), residual connection, and layer normalization. Different variations of transformers result from combining these four operations in various ways. For instance, Press et al. (2019) propose to frontload additional attention operations and backload additional MLP layers in a sandwich-like instead of interleaved way, Lu et al. (2019) prepend an MLP layer before the attention in each transformer block, So et al. (2019) use neural architecture search methods to evolve even more sophisticated transformer blocks, and so on. Various methods exist to approximate the attention operation, multiple modifications of the norm operation, and connectivity of the block; see, for example, (Lin et al., 2021) for a taxonomy of different models. At present, however, the search for new transformer architectures is driven mostly by empirical evaluations, and the theoretical principles behind this growing list of architectural variations is missing.

Additionally, the computational role of the four elements remains the subject of discussions. Originally, Vaswani et al. (2017) emphasized attention as the most important part of the transformer block, arguing that the learnable long-range dependencies are more powerful than the local inductive biases of convolutional networks. On the other hand more recent investigations (Yu et al., 2021) argue that the entire transformer block is important. The "correct" way to combine the four basic operations inside the block remains unclear, as does an understanding of the core computational function of the entire block and each of its four elements.

In a seemingly unrelated line of work, Associative Memory models, also known as Hopfield Networks (Hopfield, 1982; 1984), have been gaining popularity in the machine learning community thanks to theoretical advancements pertaining to their memory storage capacity and novel architectural modifications. Specifically, it has been shown that increasing the sharpness of the activation functions can lead to super-linear (Krotov & Hopfield, 2016) and even exponential (Demircigil et al., 2017) memory storage capacity for these models, which is important for machine learning applications. This new class of Hopfield Networks is called Dense Associative Memories or Modern

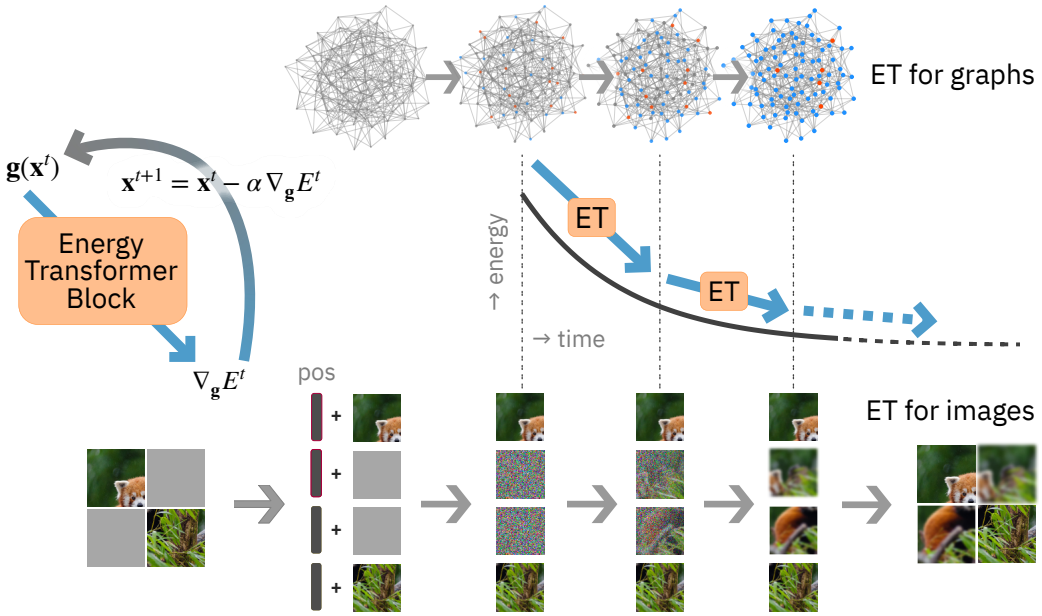

Figure 1: Overview of the Energy Transformer (ET). Instead of a sequence of conventional transformer blocks, a single recurrent ET block is used. The operation of this block is dictated by the global energy function. The token representations are updated according to a continuous time differential equation with the time-discretized update step $\alpha = dt/\tau$. On the image domain, images are split into non-overlapping patches that are linearly encoded into tokens with added learnable positional embeddings (POS). Some patches are randomly masked. These tokens are recurrently passed through ET, and each iteration reduces the energy of the set of tokens. The token representations at or near the fixed point are then decoded using the decoder network to obtain the reconstructed image. The network is trained by minimizing the mean squared error loss between the reconstructed image and the original image. On the graph domain, the same general pipeline is used. Each token represents a node, and each node has its own positional encoding. The token representations at or near the fixed point are used for the prediction of the anomaly status of each node.

Hopfield Networks. Ramsauer et al. (2020) additionally describe how the attention mechanism in transformers is closely related to a special model of this family with the $\mathrm{softmax}$ activation function.

There are high-level conceptual similarities between transformers and Dense Associative Memories, since both architectures are designed for some form of denoising of the input. Transformers are typically pre-trained on a masked-token task, e.g., in the domain of Natural Language Processing (NLP) certain tokens in the sentence are masked and the model predicts the masked tokens. Dense Associative Memory models are designed for completing the incomplete patterns. For instance, a pattern can be the concatenation of an image and its label, and the model can be trained to predict part of the input (the label), which is masked, given the query (the image). They can also be trained in a self-supervised way by predicting the occluded parts of the image, or denoising the image.

There are also high-level differences between the two classes of models. Associative Memories are recurrent networks with a global energy function so that the network dynamics converges to a fixed point attractor state corresponding to a local minimum of the energy function. Transformers are typically not described as dynamical systems at all. Rather, they are thought of as feed-forward networks built of the four computational elements discussed above. Even if one thinks about them as dynamical systems with tied weights, e.g., (Bai et al., 2019), there is no reason to expect that their dynamics converge to a fixed point attractor (see the discussion in (Lan et al., 2020)).

Additionally, a recent study (Yang et al., 2022) uses a form of Majorization-Minimization algorithms (Sun et al., 2016) to interpret the forward path in the transformer block as an optimization process. This interpretation requires imposing certain constraints on the operations inside the block, and attempting to find an energy function that describes the constrained block. We take a complementary

approach by using intuition developed in Associative Memory models to *start* with an energy function that is perfectly suited for the problem of interest. The optimization process and the resulting transformer block in our approach is a *consequence* of this specifically chosen energy function.

Concretely, we use the recent theoretical advancements and architectural developments in Dense Associative Memories to design an energy function tailored to route the information between the tokens. The goal of this energy function is to represent the relationships between the semantic contents of tokens describing a given data point (e.g., the relationships between the contents of the image patches in the vision domain, or relationships between the nodes' attributes in the graph domain). The core mathematical idea of our approach is that the sequence of these unusual transformer blocks, which we call the Energy Transformer (ET), minimizes this global energy function. Thus, the sequence of conventional transformer blocks is replaced with a single ET block, which iterates the token representations until they converge to a fixed point attractor state. In the image domain, this fixed point corresponds to the completed image with masked tokens replaced by plausible auto-completions of the occluded image patches. In the graph domain, the fixed point reveals the anomaly status of a given node given that node's neighbors; see Figure 1. The energy function in our ET block is designed with the goal to describe the *relationships between the tokens*. Examples of relationships in the image domain are: straight lines tend to continue through multiple patches, given a face with one eye being masked the network should impaint the missing eye, etc. In the graph domain, these are the relationships between the attributes and the anomaly status of the connected nodes. The optimization procedure during the forward path of ET uses continuous time differential equations, and describes a gradient decent on the specifically chosen energy function.

The core mathematical principle of the ET block – the existence of the global energy function – dictates strong constraints on the possible operations, the order in which these operations are executed in the forward path, and the symmetries of the weights in the network. As a corollary of this theoretical principle, the attention mechanism of ET is different from the attention mechanism commonly used in feed-forward transformers (Vaswani et al., 2017).

In the following section we introduce the global energy function for the ET block and explain the block's architecture. We then explore the inner workings of the ET network for image completion and qualitatively assess the learned representations (the model is trained on ImageNet-1k in a general pipeline similar to Dosovitskiy et al. (2021)). Finally, we turn to the graph anomaly detection task, which is conceptually similar to the image completion setting but has a record of strong published benchmarks against which our approach can be quantitatively compared. We show that the ET network stands in line with or outperforms the latest benchmarks. Although we focus on the computer vision and anomaly detection domains in this paper, we believe that the computational principles developed can be applied to other exciting domains (e.g., NLP, audio, and video) in which conventional transformers have shown promising results.

2 Energy Transformer Block

We now introduce the theoretical framework of the ET network. For clarity of presentation, we use language associated with the image domain. For the graph domain, one should think about "image patches" as nodes on the graph.

The overall pipeline is similar to the Vision Transformer networks (ViTs) and is shown in Figure 1. An input image is split into non-overlapping patches. After passing these patches through the encoder and adding the positional information, the semantic content of each patch and its position is encoded in the token x_{iA}. In the following the indices $i, j, k = 1...D$ are used to denote the token vector's elements, indices $A, B, C = 1...N$ are used to enumerate the patches and their corresponding tokens. It is helpful to think about each image patch as a physical particle, which has a complicated internal state described by a D-dimensional vector $\mathbf{x_A}$. This internal state describes the identity of the particle (representing the pixels of each patch), and the particle's positional embedding (the patch's location within the image). The ET block is described by a continuous time differential equation, which describes interactions between these particles. Initially, at $t = 0$ the network is given a set containing two groups of particles corresponding to open and masked patches. The "open" particles know their identity and location in the image. The "masked" particles only know where in the image they are located, but are not provided the information about what image patch they represent. The goal of ET's non-linear dynamics is to allow the masked particles to find

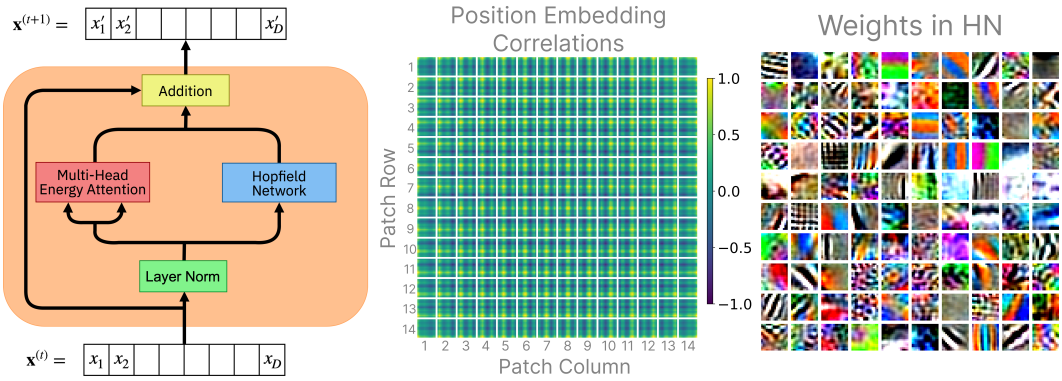

Figure 2: **Left**: Inside the ET block. The input token $\mathbf{x}$ passes through a sequence of operations and gets updated to produce the output token $\mathbf{x}'$. The operations inside the ET block are carefully engineered so that the entire network has a global energy function, which decreases with time and is bounded from below. In contrast to conventional transformers, the ET-based analogs of the attention module and the feed-forward MLP module are applied in parallel as opposed to consecutively. **Center**: The cosine similarity between the learned position embedding of each patch and every other patch. In each cell, the brightest patch indicates the cell of consideration. **Right**: 100 selected memories stored in the HN memory matrix, visualized by the decoder as 16x16 RGB image patches. This visualization is unique to our model, as traditional Transformers cannot guarantee image representations in the learned weights.

an identity consistent with their locations and the identities of open particles. This dynamical evolution is designed so that it minimizes a global energy function, and is guaranteed to arrive at a fixed point attractor state. The identities of the masked particles are considered to be revealed when the dynamical trajectory reaches the fixed point. Thus, the central question is: how can we design the energy function that accurately captures the task that the Energy Transformer needs to solve?

The masked particles' search for identity is guided by two pieces of information: identities of the open particles, and the general knowledge about what patches are in principle possible in the space of all possible images. These two pieces of information are described by two contributions to the ET's energy function: the energy based attention and the Hopfield Network, respectively, for reasons that will become clear in the next sections. Below we define each element of the ET block in the order they appear in Figure 2.

Layer Norm

Each token is represented by a vector $\mathbf{x} \in R^D$. At the same time, most of the operations inside the ET block are defined using a layer-normalized token representation

$$g_i = \gamma \frac{x_i - \bar{x}}{\sqrt{\frac{1}{D}\sum_j \left(x_j - \bar{x}\right)^2 + \varepsilon}} + \delta_i, \quad \text{where} \quad \bar{x} = \frac{1}{D}\sum_{k=1}^{D} x_k \tag{1}$$

The scalar γ and the vector δ_i are learnable parameters, ε is a small regularization constant. Importantly, this operation can be viewed as an activation function for the neurons and can be defined as a partial derivative of the Lagrangian function

$$L = D\gamma \sqrt{\frac{1}{D}\sum_j \left(x_j - \bar{x}\right)^2 + \varepsilon} + \sum_j \delta_j x_j, \quad \text{so that} \quad g_i = \frac{\partial L}{\partial x_i} \tag{2}$$

See Krotov & Hopfield (2021); Tang & Kopp (2021); Krotov (2021) for a detailed discussion of this property.

MULTI-HEAD ENERGY ATTENTION

The first contribution to the ET's energy function is responsible for exchanging information between the particles (patches). Similarly to the conventional attention mechanism, each token generates a pair of queries and keys (ET does not have a separate value matrix; instead the value matrix is a function of keys and queries). The goal of the energy based attention is to evolve the tokens in such a way that the keys of the open patches are aligned with the queries of the masked patches in the internal space of the attention operation. Below we use index $\alpha = 1...Y$ to denote elements of this internal space, and index $h = 1...H$ to denote different heads of this operation. With these notations the energy-based attention operation is described by the following energy function:

$$E^{\text{ATT}} = -\frac{1}{\beta} \sum_h \sum_C \log \left(\sum_{B \neq C} \exp \left(\beta \sum_\alpha K_{\alpha h B} \, Q_{\alpha h C} \right) \right) \tag{3}$$

where the queries and keys tensors are defined as

$$\begin{aligned} K_{\alpha h B} &= \sum_j W^K_{\alpha h j} \, g_{jB}, \qquad \mathbf{K} \in R^{Y \times H \times N} \\ Q_{\alpha h C} &= \sum_j W^Q_{\alpha h j} \, g_{jC}, \qquad \mathbf{Q} \in R^{Y \times H \times N} \end{aligned} \tag{4}$$

and the tensors $\mathbf{W}^K \in R^{Y \times H \times D}$ and $\mathbf{W}^Q \in R^{Y \times H \times D}$ are learnable parameters.

From the computational perspective each patch generates two representations: query (given the position of the patch and its current content, where in the image should it look for the prompts on how to evolve in time?), and key (given the current content of the patch and its position, what should be the contents of the patches that attend to it?). The log-sum energy function (3) is minimal when for every patch in the image its queries are aligned with the keys of a small number of other patches connected by the attention map. Different heads (index h) contribute to the energy additively.

HOPFIELD NETWORK MODULE

The next step of the ET block, which we call the Hopfield Network (HN), is responsible for ensuring that the token representations are consistent with what one expects to see in realistic images. The energy of this sub-block is defined as:

$$E^{\text{HN}} = -\frac{1}{2} \sum_{B,\mu} r\Big(\sum_j \xi_{\mu j} \, g_{jB} \Big)^2, \qquad \xi \in R^{K \times D} \tag{5}$$

where $\xi_{\mu j}$ is a set of learnable weights (memories in the Hopfield Network), and $r(\cdot)$ is an activation function. Depending on the choice of the activation function this step can be viewed either as a classical continuous Hopfield Network (Hopfield, 1984) if the activation function grows slowly (e.g., ReLU), or as a modern continuous Hopfield Network (Krotov & Hopfield, 2016; Ramsauer et al., 2020; Krotov & Hopfield, 2021) if the activation function is sharply peaked around the memories (e.g. power or softmax). The HN sub-block is analogous to the feed-forward MLP step in the conventional transformer block but requires that the weights of the projection from the token space to the hidden neuron's space to be the same (transposed matrix) as the weights of the subsequent projection from the hidden space to the token space. Thus, the HN module here is an MLP with shared weights that is *applied recurrently*. The energy contribution of this block is low when the tokens representations are aligned with some rows of the matrix ξ, which represent memories.

DYNAMICS OF TOKEN UPDATES

The forward path of the ET network is described by the continuous time differential equation, which minimizes the sum of the two energies described above

$$\tau \frac{dx_{iA}}{dt} = -\frac{\partial E}{\partial g_{iA}}, \quad \text{where} \quad E = E^{\text{ATT}} + E^{\text{HN}} \tag{6}$$

Here x_{iA} is the token representation (input and output from the ET block), and g_{iA} is its layer-normalized version. The first energy is low when each patch's queries are aligned with the keys

of its neighbors. The second energy is low when each patch has content consistent with the general expectations about what an image patch should look like (memory slots of the matrix χ). The dynamical system (6) finds a trade-off between these two desirable properties of each token's representation.

To demonstrate that the dynamical system (6) minimizes the energy, consider the temporal derivative

$$\frac{dE}{dt} = \sum_{i,j,A} \frac{\partial E}{\partial g_{iA}} \frac{\partial g_{iA}}{\partial x_{jA}} \frac{dx_{jA}}{dt} = -\frac{1}{\tau} \sum_{i,j,A} \frac{\partial E}{\partial g_{iA}} M^A_{ij} \frac{\partial E}{\partial g_{jA}} \leq 0 \tag{7}$$

The last inequality sign holds if the symmetric part of the matrix

$$M^A_{ij} = \frac{\partial g_{iA}}{\partial x_{jA}} = \frac{\partial^2 L}{\partial x_{iA} \partial x_{jA}}$$

is positive semi-definite (for each value of index A). The Lagrangian (2) satisfies this condition.

Relationship to Modern Hopfield Networks and Conventional Attention

One of the theoretical contributions of our work is the design of the energy attention mechanism and the corresponding energy function (3). Although heavily inspired by prior work on Modern Hopfield Networks, our approach is fundamentally different from it. Our energy function (3) may look somewhat similar to the energy function of a continuous Hopfield Network with the $\mathrm{softmax}$ activation function. The main difference, however, is that in order to use Modern Hopfield Networks recurrently (as opposed to applying their update rule only once) the keys must be constant parameters (called memories in the Hopfield language). In contrast, in our energy attention network the keys are dynamical variables that evolve in time with the queries.

To emphasize this further, it is instructive to write explicitly the ET attention contribution to the update dynamics (6). It is given by (for clarity, assume only one head of attention):

$$-\frac{\partial E^{\text{ATT}}}{\partial g_{iA}} = \sum_{C \neq A} \sum_{\alpha} W^Q_{\alpha i} \, K_{\alpha C} \, \underset{C}{\mathrm{softmax}}\Big(\beta \sum_{\gamma} K_{\gamma C} \, Q_{\gamma A}\Big) + W^K_{\alpha i} \, Q_{\alpha C} \, \underset{A}{\mathrm{softmax}}\Big(\beta \sum_{\gamma} K_{\gamma A} \, Q_{\gamma C}\Big)$$

In both terms the $\mathrm{softmax}$ normalization is done over the token index of the keys, which is indicated by the subscript in the equation. The first term in this formula is the conventional attention mechanism (Vaswani et al., 2017) with the value matrix equal to $\mathbf{V} = (\mathbf{W}^Q)^T \mathbf{K} = \sum_\alpha W^Q_{\alpha i} K_{\alpha C}$. The second term is the brand new contribution that is missing in the original attention mechanism. The presence of this second term is crucial to make sure that the dynamical system (6) minimizes the energy function if applied recurrently. This second term is the main difference of our approach compared to the Modern Hopfield Networks. The same difference applies to the other recent proposals (Yang et al., 2022).

Lastly, we want to emphasize that our ET block contains two different kinds of Hopfield Networks acting in parallel, see Figure 2. The first one is the energy attention module, which is inspired by, but not identical to, Modern Hopfield Networks. The second one is the "Hopfield Network" module, which can be either a classical or modern Hopfield Network. These two should not be confused.

3 Qualitative Inspection of the ET framework on ImageNet

We have trained the ET network on the masked image completion task using ImageNet-1k dataset (Deng et al., 2009). Each image was broken into non-overlapping patches of 16x16 RGB pixels, which were projected with a single affine encoder into the token space. Half of these tokens were "masked", e.g., by replacing them with a learnable MASK token. A distinct learnable position encoding vector was added to each token. Our ET block then processes all tokens recurrently for T steps. The token representations after T steps are passed to a simple linear decoder (consisting of a layer norm and an affine transformation). The loss function is the standard MSE loss on the occluded patches. See more details on the implementation and the hyperparameters in Appendix A.

Examples of occluded/reconstructed images (unseen during training) are shown in Figure 3. In general, our model learns to perform the task very well, capturing the texture in dog fur (col 3) and

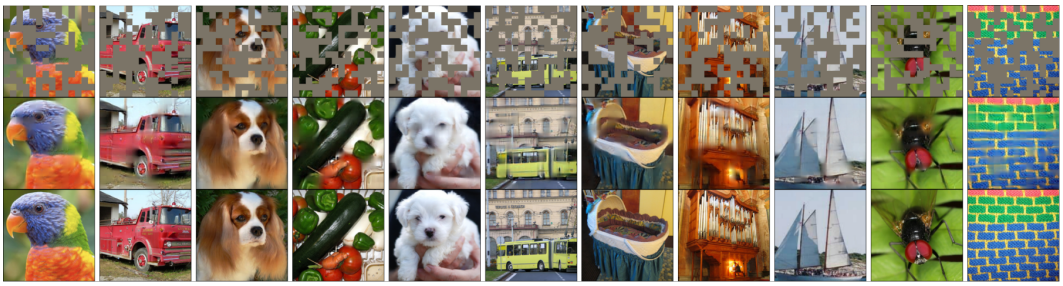

Figure 3: Reconstruction examples of our Energy Transformer using images from the ImageNet-1k validation set. *Top row:* input images where 50% of the patches are masked with the learned MASK token. *Middle row*: output reconstructions after 12 time steps. *Bottom row*: original images.

understanding meaningful boundaries of objects. However, we observe that our single ET block struggles to understand some global structure, e.g., failing to capture both eyes of the white dog (col 4) and completing irregular brick patterns in the name of extending the un-occluded borders (last col). We additionally inspect the positional encoding vectors associated with every token, Figure 2, where the model learns a locality structure in the image plane that is very similar to the original ViT (Dosovitskiy et al., 2021). The position embedding of each image patch has learned high similarity values to other patches in the same row and column, with similarity values higher for neighboring tokens than distant tokens.

Our network is unique compared to standard ViTs in that the iterative dynamics only *move* tokens around in the same space from which the final fixed point representation can be decoded back into the image plane. This functionality makes it possible to visualize essentially any *token representation*, *weight*, or *gradient of the energy* directly in the image plane. This feature is highly desirable from the perspective of interpretability, since it makes it possible to track the updates performed by the network directly in the image plane as the computation unfolds in time. In Figure 2 this functionality is used for inspecting the learned weights of the HN module directly in the image plane. According to our theory, these weights should represent basis vectors in the space of all possible image patches. These learned representations look qualitatively similar to the representations typically found in networks trained on image datasets, e.g., Zeiler & Fergus (2014).

We additionally visualize the gradients of the energy function (which are equal to the token updates, see Equation 6) of both ATTN block and the HN block, see Figure 4. Early in time, almost all signal to the masked tokens comes from the ATTN block, which routes information from the open patches to the masked ones; no meaningful signal comes from the HN block to the masked patch dynamics. Later in time we observe a different phenomenon: almost all signal to masked tokens comes from the HN module while ATTN contributes a blurry and uninformative signal. Thus, the attention layer is crucial early in the network dynamics, feeding signal to masked patches from the visible patches, whereas the HN is crucial later in the dynamics as the model approaches the final reconstruction, sharpening the masked patches. All the qualitative findings presented in this section are in accord with the core computational strategy of the ET block as it was designed theoretically in section 2.

4 Graph Anomaly Detection

Having built the theoretical foundation of the ET network and gained an intuition about its inner workings through visualizations, we turn to quantitatively evaluating its performance on the graph anomaly detection problem, a task with plenty of strong and recently published baselines. Anomalies are outliers that significantly deviate in their properties from the majority of the samples. Detecting anomalies on graphs has broad applications in cybersecurity (Hong et al., 2014; Pan et al., 2019), fraud detection (Huang et al., 2018; Pourhabibi et al., 2020), and social networks (Chaker et al., 2017). Generally, there are three types of graph anomalies: node anomaly, edge anomaly, and subgraph anomaly. In this work, we focus on node anomaly detection in attributed graphs. This task is perfectly suited for the ET network, since each node's attributes can be encoded in the latent

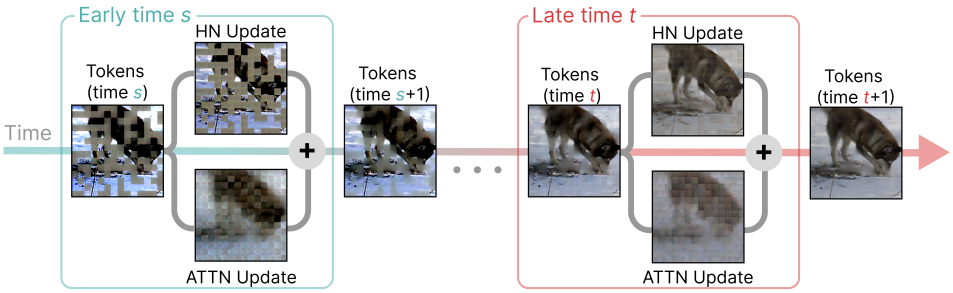

Figure 4: Token representations and gradients are visualized using the decoder at different times during the dynamics. The Energy Attention (ATTN) block contributes general structure information to the masked patches at *earlier* time steps, whereas the Hopfield Network (HN) significantly sharpens the quality of the masked patches at *later* time steps.

space and treated as a token (with added learnable positional embeddings). The network iterates these representations in time, and the outputs can be used for the node anomaly classification task.

Graph Convolutional Networks (GCN) (Kipf & Welling, 2016) have been widely used for this task due to their capability of learning high level representations of graph structures and node attributes (Ding et al., 2019; Peng et al., 2020). However, vanilla GCNs suffer from the over-smoothing problem (Wu et al., 2019). In each layer of the forward pass, the outlier node aggregates information from its neighbors. This averaging makes the features of anomalies less distinguishable from the features of benign nodes. Our approach does not suffer from this problem, since the routing of the information between the nodes is done through the energy based attention, which uses different aggregation procedure depending on whether or not the node is anomalous.

In order to turn the anomaly detection task on graphs into the ET framework, consider an undirected graph with N nodes. Every node has a vector of attributes $\mathbf{y}_A \in R^F$, where F is the number of node's features. Additionally, every node has a binary label l_A, indicating whether the node is benign or not. We focus on node anomaly and assume that all edges are trusted. The task is to predict the label of the node given the graph structure and the node's features. Since there are far more benign nodes in the graph than anomalous ones, anomaly detection can be regarded as an imbalanced node classification task.

First, the feature vectors for every node are converted to a token representation using a linear embedding $\mathbf{E}$ and adding a learnable positional embedding λ_A

$$\mathbf{x}_A^{t=0} = \mathbf{E}\mathbf{y}_A + \lambda_A$$

where the superscript 0 indicates the time of the update of the ET dynamics. This token representation is iterated through the ET block for T iterations. When the retrieval dynamics becomes stable, we have the final representation for each node $\mathbf{x}_A^{t=T}$ (or more precisely $\mathbf{g}_A^{t=T}$, since the outputs are additionally passed through a layer norm operation after the final ET update). This output is concatenated with the initial (layer normalized) token to form the final output of the network

$$\mathbf{g}_A^{\text{final}} = \mathbf{g}_A^{t=0} \,||\, \mathbf{g}_A^{t=T}$$

Following Tang et al. (2022), the node representation $\mathbf{g}_A^{\text{final}}$ is fed into an MLP with the sigmoid activation function to compute the anomaly probabilities p_A. The weighted cross entropy

$$\text{Loss} = \sum_A \Big[\sigma\, l_A \log(p_A) + (1 - l_A)\log(1 - p_A)\Big]$$

is then minimized to train the whole network. Above, σ is the ratio of anomalous labels (l_A = 1) to the regular labels (l_A = 0).

4.1 Experimental Evaluation

Four datasets are used for the graph anomaly detection experiments. YelpChi dataset (Rayana & Akoglu, 2015) aims at opinion spam detection in Yelp reviews. Amazon dataset is used to detect

anomalous users under the Musical Instrument Category on *amazon.com* (McAuley & Leskovec, 2013). T-Finance and T-Social datasets (Tang et al., 2022) are used for anomalous account detection in the transactions and social networks, respectively. For these four datasets, the graph is treated as a homogeneous graph (i.e. all the edges are of the same type), and a feature vector is associated with each node. The task is to predict the label (anomaly status) of the nodes. For each dataset, either 1% or 40% of the nodes are used for training, and the remaining 99% or 60% are split $1:2$ into validation and testing, see Appendix B for details.

We compare with state-of-the-art approaches for graph anomaly detection, which include GraphConsis (Liu et al., 2020), CAREGNN (Dou et al., 2020), PC-GNN (Liu et al., 2021) and BWGNN (Tang et al., 2022). Additionally, multi-layer perceptrons (MLP) and Graph Transformer (GT) (Dwivedi & Bresson, 2020) are included in the baselines for completeness. Following previous work, macro-F1 score (unweighted mean of F1 score) and the Area Under the Curve (AUC) are used as the evaluation metrics on the test datasets Davis & Goadrich (2006). See Appendix B for more details on training protocols and the hyperparameters choices. The results are reported in Table 1. Our ET network demonstrates very strong results across all the datasets.

Table 1: Performance of all the methods on Yelp, Amazon, T-Finance, and T-Social datasets with different training ratios. Following Tang et al. (2022), mean and standard deviation over 5 runs with different train/dev/test split are reported for our method and the baselines (standard deviations are only included if they are available in the prior work). Best results are in **bold**. Our model is state of the art or near state of the art on every category.

	Datasets	Split	GraphConsis	CAREGNN	PC-GNN	BWGNN	MLP	GT	ET (Ours)
Macro-F1	Yelp	1%	$56.8_{\pm 2.8}$	$62.1_{\pm 1.3}$	$59.8_{\pm 1.4}$	$61.1_{\pm 0.4}$	$53.9_{\pm 0.2}$	$61.7_{\pm 0.4}$	$\mathbf{63.0_{\pm 0.6}}$
		40%	$58.7_{\pm 2.0}$	$63.3_{\pm 0.9}$	$63.0_{\pm 2.3}$	$71.0_{\pm 0.9}$	$57.5_{\pm 0.8}$	$68.7_{\pm 0.4}$	$\mathbf{71.5_{\pm 0.1}}$
	Amazon	1%	$68.5_{\pm 3.4}$	$68.7_{\pm 1.6}$	$79.8_{\pm 5.6}$	$\mathbf{90.9_{\pm 0.7}}$	$74.6_{\pm 1.2}$	$88.6_{\pm 0.5}$	$89.3_{\pm 0.7}$
		40%	$75.1_{\pm 3.2}$	$86.3_{\pm 1.7}$	$89.5_{\pm 0.7}$	$92.2_{\pm 0.4}$	$79.1_{\pm 1.2}$	$91.7_{\pm 0.8}$	$\mathbf{92.8_{\pm 0.3}}$
	T-Finance	1%	71.7	73.3	62.0	84.8	61.0	81.5	$\mathbf{85.1_{\pm 1.0}}$
		40%	73.4	77.5	63.1	86.8	70.5	83.6	$\mathbf{88.2_{\pm 1.0}}$
	T-Social	1%	52.4	55.8	51.1	75.9	50.0	64.3	$\mathbf{79.1_{\pm 0.7}}$
		40%	56.5	56.2	52.1	**83.9**	50.3	68.2	$\mathbf{83.5_{\pm 0.4}}$
AUC	Yelp	1%	$66.4_{\pm 3.4}$	$75.0_{\pm 3.8}$	$\mathbf{75.4_{\pm 0.9}}$	$72.0_{\pm 0.5}$	$59.8_{\pm 0.4}$	$72.5_{\pm 0.6}$	$73.2_{\pm 0.8}$
		40%	$69.8_{\pm 3.0}$	$76.1_{\pm 2.9}$	$79.8_{\pm 0.1}$	$84.0_{\pm 0.9}$	$66.5_{\pm 1.0}$	$81.9_{\pm 0.5}$	$\mathbf{84.9_{\pm 0.3}}$
	Amazon	1%	$74.1_{\pm 3.5}$	$88.6_{\pm 3.5}$	$90.4_{\pm 2.0}$	$89.4_{\pm 0.3}$	$83.6_{\pm 1.7}$	$89.0_{\pm 1.2}$	$\mathbf{91.9_{\pm 1.0}}$
		40%	$87.4_{\pm 3.3}$	$90.5_{\pm 1.6}$	$95.8_{\pm 0.1}$	$98.0_{\pm 0.4}$	$89.8_{\pm 1.0}$	$95.4_{\pm 0.6}$	$\mathbf{97.3_{\pm 0.4}}$
	T-Finance	1%	90.2	90.5	90.7	91.1	82.9	90.0	$\mathbf{92.8_{\pm 1.1}}$
		40%	91.4	92.1	91.2	94.3	87.1	88.2	$\mathbf{95.0_{\pm 3.0}}$
	T-Social	1%	65.2	71.2	59.8	88.0	56.3	81.4	$\mathbf{91.9_{\pm 0.6}}$
		40%	71.2	71.8	68.4	**95.2**	56.9	82.5	$93.9_{\pm 0.2}$

5 Discussion and Conclusions

A lot of recent research has been dedicated to understanding the striking analogy between Hopfield Networks and the attention mechanism in transformers. At a high level, the main message of our work is that the *entire* transformer block (including feed-forward MLP, layer normalization, and residual connections) can be viewed as a single large Hopfield Network, not just attention alone. At a deeper level, we use recent advances in the field of Hopfield Networks to design a novel energy function that is tailored for dynamical information routing between the tokens and representation of a large number of relationships between those tokens. When used in the encoder-decoder setting, an appealing feature of our network is that any state, weight, or state update can be mapped directly into the data domain. This provides the possibility to inspect the inner workings of the whole network, contributing to its interpretability. The attention mechanism in our network contains an important extra term compared to conventional attention. We have tested the ET network on the image completion task (qualitatively) and node anomaly detection on graphs (quantitatively). The qualitative investigation reveals the perfect alignment between the theoretical design principles of our network and its empirical computation. The quantitative evaluation demonstrates strong results, which stand in line or exceed the methods recently developed specifically for this task. Although we have only tested ET on two tasks, we intentionally picked two entirely different data domains (images and graphs). We believe that the proposed network will be useful for other tasks and domains and deserves a comprehensive investigation in line with other popular variants of transformers.

6 REPRODUCIBILITY STATEMENT

Section does not count towards page limit

In the experiments presented in this paper we have taken several steps to ensure reproducibility of our results. Namely, all the training protocols and implementation details including the hyperparameter selection are described in Appendix A and Appendix B. All code is on GitHub and awaiting the paper's acceptance to be released (we can also release it during the discussion period for ther use by the reviewers). The code for image reconstruction is written in JAX Bradbury et al. (2018) with a single entry script to launch the training process, with defaults set to the configuration that produced the models used in this paper. The training script sets a seed that can recreate the exact same training setup as we had, ensuring the exact same weight initialization and random data augmentation provided default arguments. No additional training data was used beyond the training set (ImageNet-1k 2012), which is publicly available. The code for Graph Anomaly Detection is written in PyTorch. Given the nature of the anomaly detection problem (random splits into training, validation, testing sets) all our results on graphs are reported with mean and standard deviations, describing typical variability in the performance.

REFERENCES

Shaojie Bai, J Zico Kolter, and Vladlen Koltun. Deep equilibrium models. *Advances in Neural Information Processing Systems*, 32, 2019.

James Bradbury, Roy Frostig, Peter Hawkins, Matthew James Johnson, Chris Leary, Dougal Maclaurin, George Necula, Adam Paszke, Jake VanderPlas, Skye Wanderman-Milne, and Qiao Zhang. JAX: Composable transformations of Python+NumPy programs, 2018.

Rima Chaker, Zaher Al Aghbari, and Imran N Junejo. Social network model for crowd anomaly detection and localization. *Pattern Recognition*, 61:266–281, 2017.

Jesse Davis and Mark Goadrich. The relationship between precision-recall and roc curves. In *Proceedings of the 23rd international conference on Machine learning*, pp. 233–240, 2006.

Mete Demircigil, Judith Heusel, Matthias Löwe, Sven Upgang, and Franck Vermet. On a model of associative memory with huge storage capacity. *Journal of Statistical Physics*, 168(2):288–299, May 2017. ISSN 1572-9613. doi: 10.1007/s10955-017-1806-y. URL `http://dx.doi.org/10.1007/s10955-017-1806-y`.

Jia Deng, Wei Dong, Richard Socher, Li-Jia Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale hierarchical image database. In *2009 IEEE conference on computer vision and pattern recognition*, pp. 248–255. Ieee, 2009.

Kaize Ding, Jundong Li, Rohit Bhanushali, and Huan Liu. Deep anomaly detection on attributed networks. In *Proceedings of the 2019 SIAM International Conference on Data Mining*, pp. 594–602. SIAM, 2019.

Kaize Ding, Jundong Li, Nitin Agarwal, and Huan Liu. Inductive anomaly detection on attributed networks. In *Proceedings of the Twenty-Ninth International Conference on International Joint Conferences on Artificial Intelligence*, pp. 1288–1294, 2021.

Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, and Neil Houlsby. An image is worth 16x16 words: Transformers for image recognition at scale. In *International Conference on Learning Representations*, 2021. URL `https://openreview.net/forum?id=YicbFdNTTy`.

Yingtong Dou, Zhiwei Liu, Li Sun, Yutong Deng, Hao Peng, and Philip S Yu. Enhancing graph neural network-based fraud detectors against camouflaged fraudsters. In *Proceedings of the 29th ACM International Conference on Information & Knowledge Management*, pp. 315–324, 2020.

Vijay Prakash Dwivedi and Xavier Bresson. A generalization of transformer networks to graphs. *arXiv preprint arXiv:2012.09699*, 2020.

Jonathan Heek, Anselm Levskaya, Avital Oliver, Marvin Ritter, Bertrand Rondepierre, Andreas Steiner, and Marc van Zee. Flax: A neural network library and ecosystem for JAX, 2020. URL http://github.com/google/flax.

Junho Hong, Chen-Ching Liu, and Manimaran Govindarasu. Integrated anomaly detection for cyber security of the substations. *IEEE Transactions on Smart Grid*, 5(4):1643–1653, 2014.

John J Hopfield. Neural networks and physical systems with emergent collective computational abilities. *Proceedings of the national academy of sciences*, 79(8):2554–2558, 1982.

John J Hopfield. Neurons with graded response have collective computational properties like those of two-state neurons. *Proceedings of the national academy of sciences*, 81(10):3088–3092, 1984.

Dongxu Huang, Dejun Mu, Libin Yang, and Xiaoyan Cai. Codetect: Financial fraud detection with anomaly feature detection. *IEEE Access*, 6:19161–19174, 2018.

Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *arXiv preprint arXiv:1609.02907*, 2016.

Dmitry Krotov. Hierarchical associative memory. *arXiv preprint arXiv:2107.06446*, 2021.

Dmitry Krotov and John J. Hopfield. Dense associative memory for pattern recognition. In D. Lee, M. Sugiyama, U. Luxburg, I. Guyon, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*, volume 29. Curran Associates, Inc., 2016. URL https://proceedings.neurips.cc/paper/2016/file/eaae339c4d89fc102edd9dbdb6a28915-Paper.pdf.

Dmitry Krotov and John J. Hopfield. Large associative memory problem in neurobiology and machine learning. In *International Conference on Learning Representations*, 2021. URL https://openreview.net/forum?id=X4y_10OX-hX.

Zhenzhong Lan, Mingda Chen, Sebastian Goodman, Kevin Gimpel, Piyush Sharma, and Radu Soricut. Albert: A lite bert for self-supervised learning of language representations. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=H1eA7AEtvS.

Tianyang Lin, Yuxin Wang, Xiangyang Liu, and Xipeng Qiu. A survey of transformers. *arXiv preprint arXiv:2106.04554*, 2021.

Yang Liu, Xiang Ao, Zidi Qin, Jianfeng Chi, Jinghua Feng, Hao Yang, and Qing He. Pick and choose: a gnn-based imbalanced learning approach for fraud detection. In *Proceedings of the Web Conference 2021*, pp. 3168–3177, 2021.

Zhiwei Liu, Yingtong Dou, Philip S Yu, Yutong Deng, and Hao Peng. Alleviating the inconsistency problem of applying graph neural network to fraud detection. In *Proceedings of the 43rd international ACM SIGIR conference on research and development in information retrieval*, pp. 1569–1572, 2020.

Yiping Lu, Zhuohan Li, Di He, Zhiqing Sun, Bin Dong, Tao Qin, Liwei Wang, and Tie-Yan Liu. Understanding and improving transformer from a multi-particle dynamic system point of view. *arXiv preprint arXiv:1906.02762*, 2019.

Julian John McAuley and Jure Leskovec. From amateurs to connoisseurs: modeling the evolution of user expertise through online reviews. In *Proceedings of the 22nd international conference on World Wide Web*, pp. 897–908, 2013.

Kaikai Pan, Peter Palensky, and Peyman Mohajerin Esfahani. From static to dynamic anomaly detection with application to power system cyber security. *IEEE Transactions on Power Systems*, 35(2):1584–1596, 2019.

Zhen Peng, Minnan Luo, Jundong Li, Luguo Xue, and Qinghua Zheng. A deep multi-view framework for anomaly detection on attributed networks. *IEEE Transactions on Knowledge and Data Engineering*, 2020.

Tahereh Pourhabibi, Kok-Leong Ong, Booi H Kam, and Yee Ling Boo. Fraud detection: A systematic literature review of graph-based anomaly detection approaches. *Decision Support Systems*, 133:113303, 2020.

Ofir Press, Noah A Smith, and Omer Levy. Improving transformer models by reordering their sublayers. *arXiv preprint arXiv:1911.03864*, 2019.

Hubert Ramsauer, Bernhard Schäfl, Johannes Lehner, Philipp Seidl, Michael Widrich, Thomas Adler, Lukas Gruber, Markus Holzleitner, Milena Pavlović, Geir Kjetil Sandve, et al. Hopfield networks is all you need. *arXiv preprint arXiv:2008.02217*, 2020.

Shebuti Rayana and Leman Akoglu. Collective opinion spam detection: Bridging review networks and metadata. In *Proceedings of the 21th acm sigkdd international conference on knowledge discovery and data mining*, pp. 985–994, 2015.

David So, Quoc Le, and Chen Liang. The evolved transformer. In *International Conference on Machine Learning*, pp. 5877–5886. PMLR, 2019.

Ying Sun, Prabhu Babu, and Daniel P Palomar. Majorization-minimization algorithms in signal processing, communications, and machine learning. *IEEE Transactions on Signal Processing*, 65 (3):794–816, 2016.

Fei Tang and Michael Kopp. A remark on a paper of krotov and hopfield [arxiv: 2008.06996]. *arXiv preprint arXiv:2105.15034*, 2021.

Jianheng Tang, Jiajin Li, Ziqi Gao, and Jia Li. Rethinking graph neural networks for anomaly detection. *arXiv preprint arXiv:2205.15508*, 2022.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in neural information processing systems*, 30, 2017.

Ross Wightman. Pytorch image models. `https://github.com/rwightman/pytorch-image-models`, 2019.

Felix Wu, Amauri Souza, Tianyi Zhang, Christopher Fifty, Tao Yu, and Kilian Weinberger. Simplifying graph convolutional networks. In *International conference on machine learning*, pp. 6861–6871. PMLR, 2019.

Yongyi Yang, Zengfeng Huang, and David Wipf. Transformers from an optimization perspective. *arXiv preprint arXiv:2205.13891*, 2022.

Weihao Yu, Mi Luo, Pan Zhou, Chenyang Si, Yichen Zhou, Xinchao Wang, Jiashi Feng, and Shuicheng Yan. Metaformer is actually what you need for vision. *arXiv preprint arXiv:2111.11418*, 2021.

Matthew D Zeiler and Rob Fergus. Visualizing and understanding convolutional networks. In *European conference on computer vision*, pp. 818–833. Springer, 2014.

Tong Zhao, Chuchen Deng, Kaifeng Yu, Tianwen Jiang, Daheng Wang, and Meng Jiang. Error-bounded graph anomaly loss for gnns. In *Proceedings of the 29th ACM International Conference on Information & Knowledge Management*, pp. 1873–1882, 2020.

A Details of Training on ImageNet

We trained the ET network on a masked-image completion task on the ImageNet-1k (IN1K) dataset. We treat all images in IN1K as images of shape 224×224 that are normalized according to standard IN1K practices (mean 0, variance 1 on the channel dimension) and use data augmentations provided by the popular `timm` library (Wightman, 2019) (See Table 2). Following the conventional ViT pipeline (Dosovitskiy et al., 2021), we split these images into non-overlapping patches of 16x16 RGB pixels which are then projected with a single affine encoder into the token dimension D for a total of 196 encoded tokens per image. We proceed to randomly and uniformly assign 100 of these

tokens as "occluded" which are the only tokens considered by the loss function. "Occluded" tokens are designated as follows: of the 100 tokens, 90 tokens are replaced with a learnable MASK token of dimension D and 10 we leave untouched (which we find important for the HN to learn meaningful patch representations). To all tokens we then add a distinct learnable position bias.

These tokens are then passed to our Energy Transformer block which we recur for T steps (the "depth" of the model in conventional Transformers). At each step, the feedback signal (the sum of the energy gradients from our attention block and HN block) is subtracted from our original token representation with a scalar step size $\alpha = \frac{dt}{\tau}$ which we treat as a non-learnable hyperparameter in our experiments. The token representations after T steps are passed to a simple linear decoder (consisting of a layer norm and an affine transformation) to project our representations back into the image plane. We then use the standard MSE Loss between the original pixels and reconstructed pixels for only the 100 occluded patches. We allow self attention as in the following formula for the energy of multiheaded attention.

$$E^{\text{ATT}} = \sum_h -\frac{1}{\beta} \sum_C \log \left(\sum_B \exp \left(\beta \sum_\alpha K_{\alpha h B} \, Q_{\alpha h C} \right) \right)$$

We give details of our architectural choices in Table 2. In the main paper we present our Energy Transformer with a configuration similar to the standard base Transformer configuration (e.g., token dimension 768, 12 heads each with $Y = 64$, softmax's $\beta = \frac{1}{\sqrt{Y}}, \ldots$), with several considerations learned from the qualitative image evaluations:

- The $\frac{dt}{\tau}$ (step size) of 1 implicitly used in the traditional transformer noticeably degrades our ability to smoothly descend the energy function. We find that a step size of 0.1 provides a smoother descent down the energy function and benefits the image reconstruction quality.
- We observe that our MSE loss must include some subset of un-occluded patches in order for the HN to learn meaningful filters.
- Values of β in the energy attention that are too high prevent our model from training. This is possibly due to vanishing gradients in our attention operation from a `softmax` operation that is too spiky.
- Without gradient clipping, our model fails to train at the learning rates we tried higher than 1e-4. We observe that gradient clipping not only helps our model train faster at the trainable learning rates, it also allows us to train at higher learning rates.

Our architecture and experiments for the image reconstruction task were written in JAX (Bradbury et al., 2018) using Flax (Heek et al., 2020). This engineering choice means that our architecture definitions are quite lightweight, as we can define the desired energy function of the ET and use JAX's autograd to automatically calculate the desired update. All training code and software will be released upon the paper's acceptance.

Table 2: Hyperparameter, architecture, and data augmentation choices for ET-base during ImageNet-1k masked training experiments. Data augmentations are listed as parameters passed to the equivalent `timm` dataloader functionality.

Training	
batch_size	768
epochs	100
lr	5e-4
warmup_epochs	2
start & end lr	5e-7
b1, b2 (ADAM)	0.9, 0.99
weight_decay	0.05
grad_clipping	1.

Architecture	
token_dim	768
num_heads	12
head_dim	64
β	1/8
train_betas	No
step size α	0.1
depth	12
hidden_dim HN	3072
bias in HN	None
bias in ATT	None
bias in LNORM	Yes

Data Augmentation	
random_erase	None
horizontal_flip	0.5
vertical_flip	0
color_jitter	0.4
scale	(0.08, 1)
ratio	(3/4, 4/3)
auto_augment	None

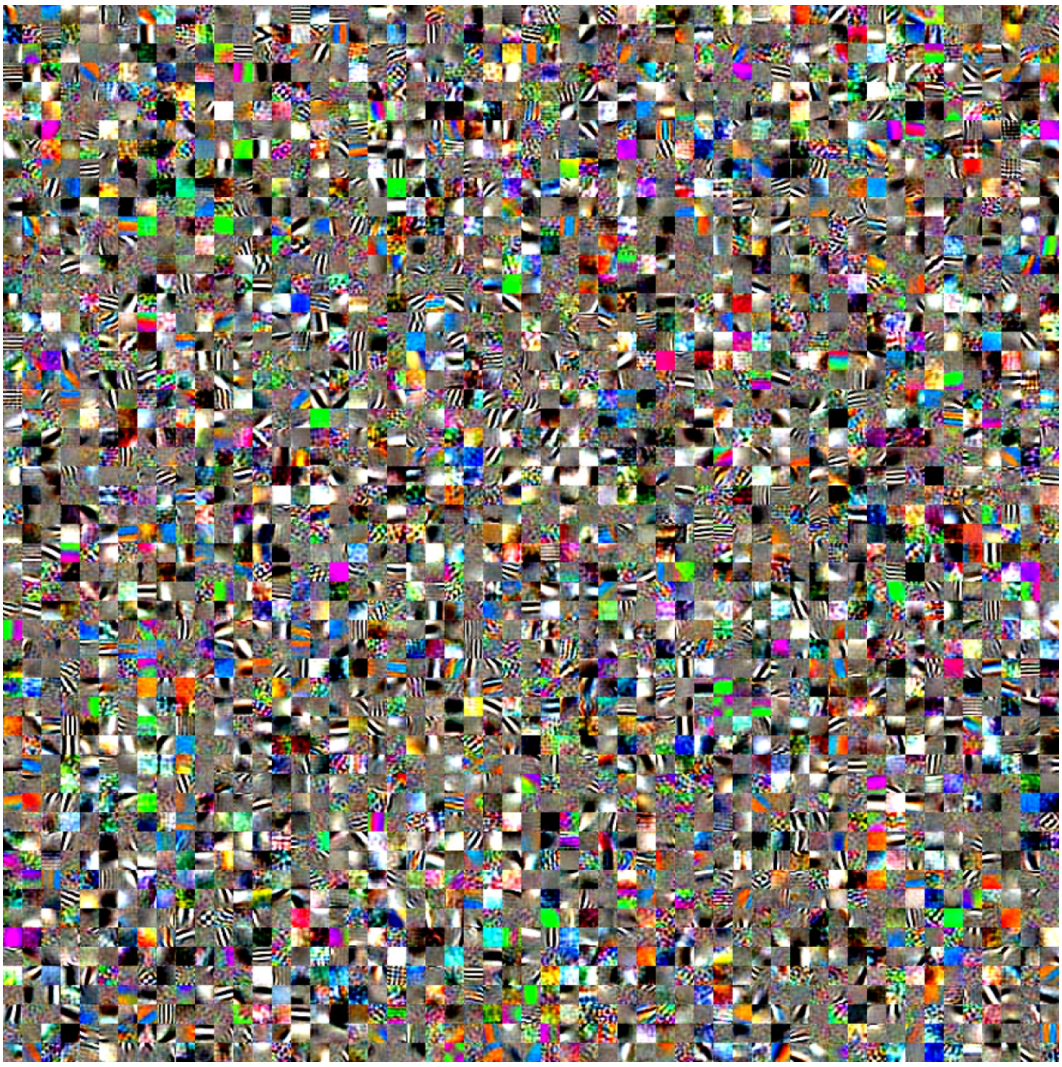

Figure 5: Visualizing a randomly selected 3025 patch memories of the 3072 learned by weight matrix in the Hopfield Network module (HN) of our model. These memories are vectors of the same dimensions D as the patch tokens, stored as rows in the weight matrix ξ. Each image patch is visualized using the model's trained decoder.

A.1 Exploring the Hopfield Memories

A distinctive aspect of our network is that any variable that has a vector index i of tokens can be mapped into the data domain by applying the decoder network to this variable. This makes it possible to inspect all the weights in the model. For instance, the concept of "memories" is crucial to understanding how Hopfield networks function. The memories within the HN module represent the building blocks of *all possible image patches* in our data domain, where an encoded image patch is a superposition of a subset of memories. The complete set of memory vectors from the HN module is shown in Figure 5. The same analysis can be applied to the weights of the ET-attention module. In Figure 6, we show all the weights from this module mapped into the image plane.

A.2 Bias Correlations

The relationships between our position embeddings exhibit similar behavior to the position correlations of the original ViT in that they are highly susceptible to choices of the hyperparameters (Figure 10 of Dosovitskiy et al. (2021)). In particular, we consider the effect of weight decay and the β pa-

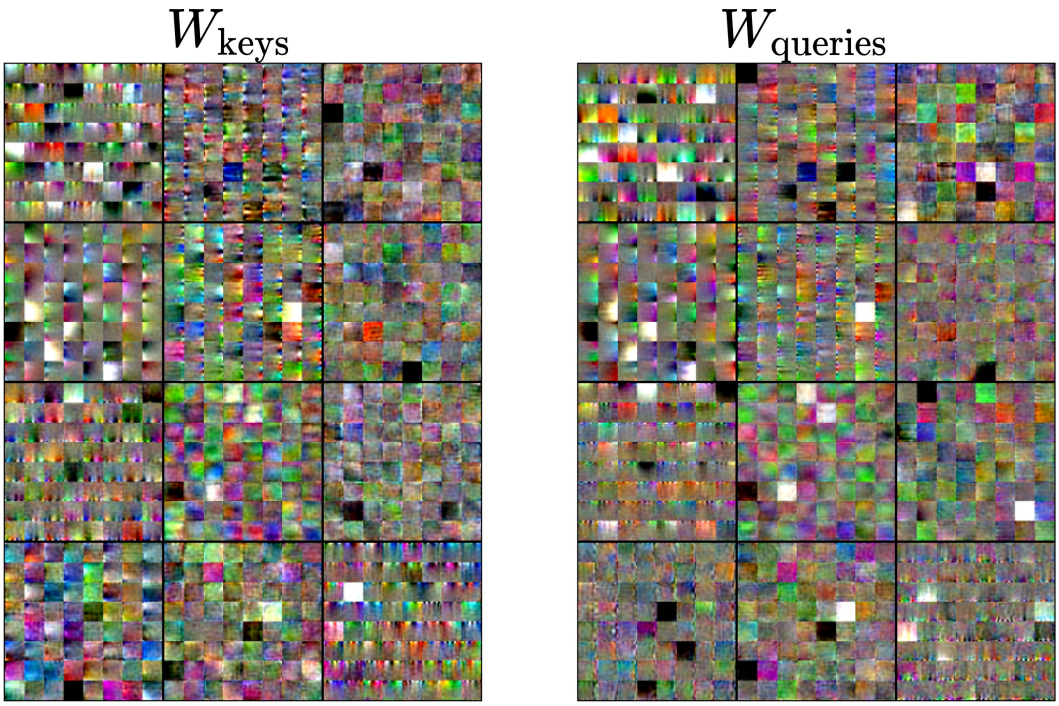

Figure 6: Visualizing the token dimension of the "key" and "query" matrices of the attention as image patches. Each head is represented as a cell on the 4×3 grid above. We use the trained decoder of our model to visualize each weight.

rameter that serves as the inverse temperature of the attention operation (see Equation 3). The lower the temperature (i.e., the higher the value of β), the spikier the softmax distribution. By using a lower β, we encourage the attention energy to distribute its positional embeddings across a wider range of patches in the model.

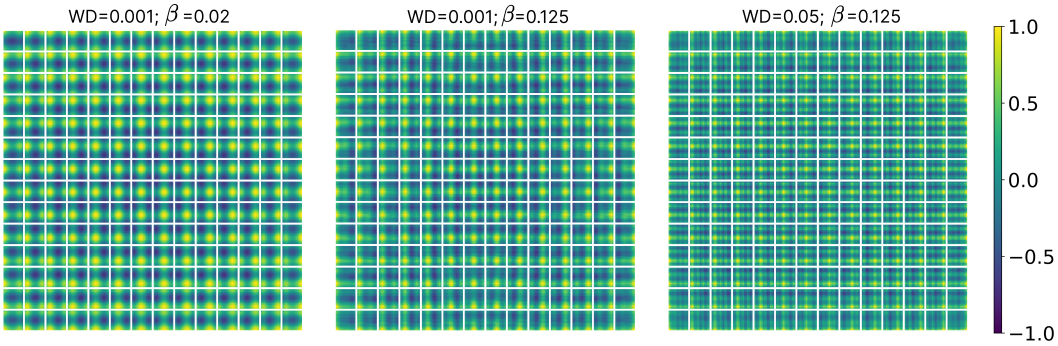

Figure 7: The cosine similarity between position biases of patches when the ET-base model is trained under different hyperparameter choices for β (inverse temperature of the attention energy) and weight decay. Our ET sees a trend where smoother correlations are observed with smaller β and weight decay.

A.3 Observing Energy Dynamics

We include as part of our supplemental submission a video showing the dynamics of one of our trained models through time together with the corresponding energy at every step. From the video, it is clear that the image progressively improves in quality as the energy decreases up to the point when the token representations are passed to the decoder. At the same time, we found it challenging

to find the time constants and number of training steps so that the energy of each image reaches the energy minimum (fixed point) when the loss is computed. For instance, for the image shown in the video, its quality actually starts to degrade when the dynamics is allowed to run for longer than what was used at training (while the energy is still decreasing). Additionally, when training models at greater depth the gradients can vanish since many recurrent applications of the ET block are necessary. We hope to comprehensively investigate these questions/limitations in future work. We include a screenshot of the video in Figure 8 and encourage readers to watch the full video for the dynamics.

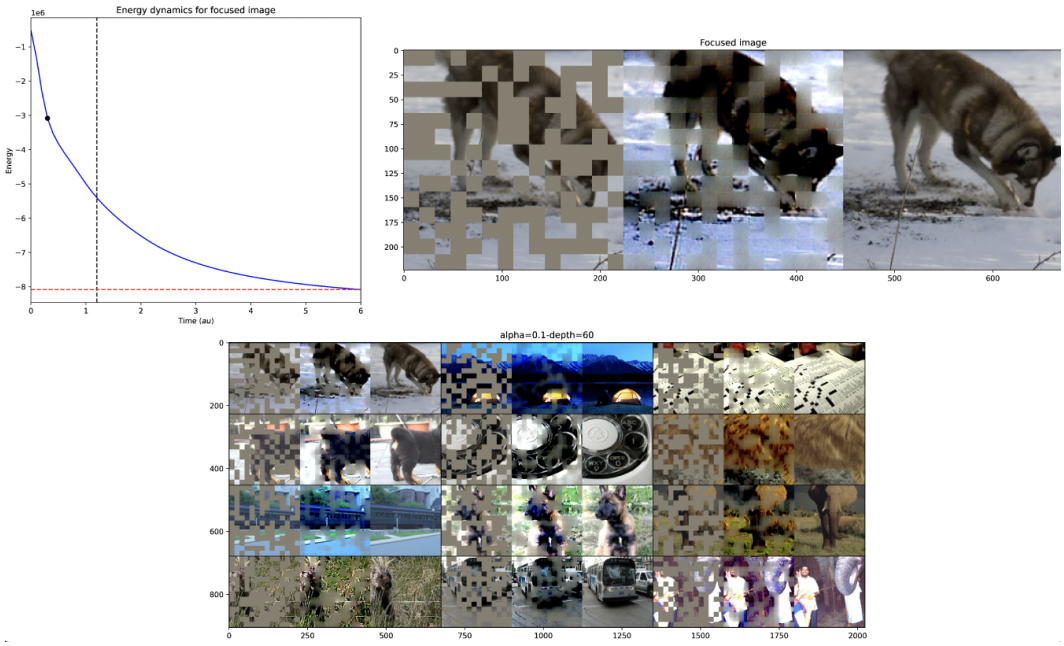

Figure 8: Screenshot of the accompanying video showcasing the energy dynamics of our model. *Top left*: the energy of our model over time (with units τ) for the dog image highlighted at the *top right*. Each cell of the dog represents the (masked input, reconstructed image at time t, original image). We step through time using a time step of $dt = 0.1$ and record the total energy of our system on the image tokens as the black dot descending the blue energy curve. The dashed vertical black line shows the point in the energy curve where the representations were passed to the loss function when training the model, whereas the horizontal red dashed line shows the "fixed point" at the end of the simulated dynamics (in reality, the energy still descends slightly after that). *Bottom:* We display 11 other images as (masked image, reconstructed image at time t, original image) aligned with the time step. Each image's energy trajectory will be slightly different (not shown).

B DETAILS OF ET TRAINING ON ANOMALY DETECTION TASK

Graph anomaly detection refers to the process of detecting outliers that deviate significantly from the majority of the samples. Neural network based methods are very popular due to their capability of learning sophisticated data representations. DOMINANT (Ding et al., 2019) utilizes an auto-encoder framework, using a GCN as an encoder and two decoders for structural reconstruction and attribute reconstruction. ALARM (Peng et al., 2020) aggregates the encoder information from multiple view of the node attributes. Another study Zhao et al. (2020), propose a novel loss function to train graph neural networks for anomaly-detectable node representations. In Ding et al. (2021) generative adversarial learning is used to detect anomaly nodes where a novel layer is designed to learn the anomaly-aware node representation. Recently, Tang et al. (2022) pointed out that anomalies can lead to the "rightshift" of the spectral energy distribution – the spectral energy concentrates more on the high frequencies. They designed a filter that can better handle this phenomenon. We propose a new anomaly detection model from the perspective of Associative Memory (pattern matching), which does not have the over-smoothing problem often faced by GCNs, and has better model interpretability (outliers should be far from the common pattern).

B.1 DETAILED MODEL STRUCTURE FOR THE GRAPH ANOMALY DETECTION

First, we compute the features that are passed to our energy-based transformer. Each node's features $\mathbf{y}_A \in R^F$ are mapped into the token space $\mathbf{x}_A \in R^D$, using a linear projection $\mathbf{E}$. Learnable positional embeddings λ_A are added to this token at $t = 0$,

$$\mathbf{x}_A^{t=0} = \mathbf{E}\mathbf{y}_A + \lambda_A$$

At each time step the input to the ET-block is layer normalized:

$$\mathbf{g}_A^t = \text{LayerNorm}(\mathbf{x}_A^t)$$

Let $\mathbf{W}^Q \in R^{Y\times H\times D}$ and $\mathbf{W}^K \in R^{Y\times H\times D}$ be the query and key weight matrices, respectively. Here Y is the projection dimension in the attention operation, H is the number of heads. We define

$$\begin{aligned} K_{\alpha hB} &= \sum_j W^K_{\alpha hj}\, g_{jB} \\ Q_{\alpha hC} &= \sum_j W^Q_{\alpha hj}\, g_{jC} \end{aligned} \tag{8}$$

If we let h indicate the index of the head, we have

$$\Delta x^t_{iA} = \sum_{C\in\mathcal{N}_A}\sum_{h,\alpha}\Big[W^Q_{\alpha hi}\, K_{\alpha hC}\, \omega_{CA} + W^K_{\alpha hi}\, Q_{\alpha hC}\, \omega_{AC}\Big] + \sum_\mu \xi_{\mu i}\, r\Big(\sum_j\, \xi_{\mu j} g_{jA}\Big)$$

where

$$\omega_{CA} = \underset{C}{\text{softmax}}\Big(\beta \sum_\gamma K_{\gamma hC}\, Q_{\gamma hA}\Big)$$

Here β controls the temperature of the softmax, $\mathcal{N}_A$ stands for the neighbors of node A – a set of all the nodes connected to node A, r is the ReLU function. Finally, we have residual connection

$$\mathbf{x}_A^{t+1} = \mathbf{x}_A^t + \mathbf{\Delta}\mathbf{x}_A^t$$

Intuitively, the first term considers the influence (attention score) of the neighbor nodes with respect to the target node, the second term considers the influence of the target node with respect to each of its neighbor, and the third term is the contribution of the Hopfield Network module. It can be shown that the forward pass of our energy-based transformer layer minimizes the following energy function:

$$E = -\frac{1}{\beta}\sum_C\sum_h \log\left(\sum_{B\in\mathcal{N}_C} \exp\left(\beta\sum_\alpha K_{\alpha hB}\, Q_{\alpha hC}\right)\right) - \frac{1}{2}\sum_{C,\mu} r\Big(\sum_j \chi_{\mu j}\, g_{jC}\Big)^2 \tag{9}$$

This energy function will decrease as the forward pass progresses until it reaches a local minimum.

After T iterations when the retrieval is stable, we have the final representation for each node $\mathbf{g}_A^{\text{final}}$ as

$$\mathbf{g}_A^{\text{final}} = \mathbf{g}_A^{t=0} \,||\, \mathbf{g}_A^{t=T}$$

where $||$ is the concatenation sign. Following Tang et al. (2022), we treat anomaly detection as semi-supervised learning task in this work. The node representation $\mathbf{g}_A^{\text{final}}$ is fed to another MLP with the sigmoid function to compute the abnormal probability p_A, weighted cross entropy is then used to train the network. The loss function is as follow:

$$\text{Loss} = \sum_A \Big[\sigma l_A \log(p_A) + (1 - l_A) \log(1 - p_A)\Big]$$

where σ is the ratio of anomaly labels (l_A = 1) to normal labels (l_A = 0).

B.2 Experimental Details

We train all models for 100 epochs using the Adam optimizer with a learning rate of 0.001, and use the model with the best Macro-F1 on the validation set for reporting the final results on the test set. Following Tang et al. (2022), we use training ratios 1% and 40% respectively (randomly select 1% and 40% nodes of the dataset to train the model, and use the remaining nodes for the validation and testing). These remaining nodes are split 1:2 for validation:testing. The statistics of the datasets are listed in Table 3. For the four datasets used in the experiments, Amazon and Yelp datasets can be obtained from the DGL library, T-Finance and T-Social can be obtained from Tang et al. (2022).

Dataset	$\|V\|$	$\|E\|$	Anomaly(%)	Features
Amazon	11944	4398392	6.87%	25
Yelp	45954	3846979	14.53%	32
T-Finance	39357	21222543	4.58%	10
T-Social	5781065	73105508	3.01%	10

Table 3: Summary of all the datasets.

We report the average performance of 5 runs on the test datasets. The hyperparameters of our model are tuned based on the validation set, selecting the best parameters within 100 epochs. To speedup the training process, for the large graph datasets T-Finance and T-Social, we sample a different subgraph to train for each epoch (subgraphs have 5% of the nodes with respect to the whole training data). The hyperparameters include the number of hidden dimensions in ET-attention Y, the number of neurons K in the hidden layer within the Hopfield Network Module, the number of time iterations T, and the number of heads H. The weights are learned via backpropagation, which includes embedding projection $\mathbf{E}$, positional embedding λ_A, softmax inverse temperature parameter β, ET-attention weight tensors $\mathbf{W}^Q$ and $\mathbf{W}^K$. The optimal hyperparameters used in Table 1 are reported in Table 4. The last row in that table summarizes the range of the hyperparameter search that was performed in our experiments. In general, we have observed that for small datasets (Yelp, Amazon, T-Finance) a 1 or 2 applications of our network is sufficient for achieving strong results, for larger datasets (T-Social) more iterations (3) are necessary. For even bigger dataset (ImageNet) our network needs about 12 iterations.

Dataset	Y	K	T	H
Amazon (40%)	128	640	1	2
Amazon (1%)	64	128	1	1
Yelp (40%)	128	256	1	1
Yelp (1%)	128	256	1	1
T-Finance (40%)	128	256	1	3
T-Finance (1%)	128	256	1	1
T-Social (40%)	128	256	3	3
T-Social (1%)	128	256	3	3
Range of hyperparameters	{64, 128, 256}	{2Y, 3Y, 4Y, 5Y}	{1,2,3}	{1,2,3}

Table 4: Hyperparameters choice of our method on all the datasets.

C NOTATIONS

Table 5 lists all the notations used in this paper.

Notations	Descriptions
F	dimension of node's feature space
D	dimension of token space
N	number of tokens
Y	number of hidden dimensions in the attention
T	number of recurrent time steps
H	number of heads
$\mathbf{y}_A$	input feature vector of node A
$\mathbf{x}_A$	vector representation of token A
x_{iA}	each element of vector representation of token A
$\mathbf{g}_A$	vector representation of token A after layernorm
g_{iA}	each element of vector representation of token A after layernorm
$\mathbf{K}$	key tensor
$\mathbf{Q}$	query tensor
$K_{\alpha hB}$	each element of the key tensor $\mathbf{K}$
$Q_{\alpha hC}$	each element of the query tensor $\mathbf{Q}$
l_A	label of node A on graph

Table 5: Notations used in the paper.