Neural Networks on Random Graphs

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Abstract

We performed a massive evaluation of neural networks with architectures corresponding to random graphs of various types. Apart from the classical random graph families including random, scale-free and small-world graphs, we introduced a novel and flexible algorithm for directly generating random directed acyclic graphs (DAG) and studied a class of graphs derived from functional resting state fMRI networks. A majority of the best performing networks were indeed in these new families. We also proposed a general procedure for turning a graph into a DAG necessary for a feed-forward neural network. We investigated various structural and numerical properties of the graphs in relation to neural network test accuracy. Since none of the classical numerical graph invariants by itself seems to allow to single out the best networks, we introduced new numerical characteristics that selected a set of quasi-1-dimensional graphs, which were the majority among the best performing networks.

1. Introduction

The main aim of this paper was to perform a wide ranging study of neural networks based on a variety of random graphs. The motivation for this study is twofold. On the one hand, artificial neural networks typically have a quite rigid connectivity structure. Yet in recent years significant advances in performance have been made through novel global architectural changes like ResNets, (He et al., 2016) or DenseNets (Huang et al., 2017). This has been further systematically exploited in the field of Neural Architecture Search (NAS, see (Elsken et al., 2019) for a review) using, among others, algorithms based on reinforcement learning (Zoph & Le, 2017; Baker et al., 2016), evolutionary techniques (Real et al., 2019) or differentiable methods (Liu et al., 2019). Hence there is a definite interest in exploring a wide variety of possible global network structures.

On the other hand, biological neural networks in the brain do not have a rigid structure and some randomness is an inherent feature of networks which evolved ontogenetically. Contrarily, we also do not expect these networks to be totally random. Therefore, it is very interesting to investigate the interrelations of structural randomness and global architectural properties with the network performance.

In the present paper, we are not focusing on optimizing the performance of a neural network (like in NAS) but rather on exploring a wide variety of random graph architectures in order to identify what features of the graph are related to good or bad performance of the associated neural network.

We performed a massive empirical study of around 1000 graphs on CIFAR-10 and CIFAR-100 datasets. Apart from the main classical families of random graphs, we introduced a novel and flexible way of generating random directed acyclic graphs (DAG) and also investigated a set of graphs derived from functional fMRI networks from Human Connectome Project data (Van Essen et al., 2013).

The paper is organized as follows. First, we discuss the relation to previous work. Next, we describe the construction of the neural network architecture associated with a given directed acyclic graph. In section 4, we describe in more detail the space of graphs that we consider and describe some of our new contributions like a principled way of passing from a graph to a DAG, as well as a construction of a flexible family of random DAGs. Here we also review the construction of graphs associated with functional fMRI networks. Section 5 contains our key results, including some a priori unexpected observations, the identification of the best networks and the introduction of novel numerical invariants which pick out the majority of the best performing graphs. We close the paper with a summary and outlook.

2. Related Work

Apart from the papers quoted already in the introduction, we would like to explicitly emphasize here further prior work incorporating randomness and irregularity in a crucial way.

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The work (Shafiee et al., 2016) proposed stochastic connections between consecutive feed-forward layers, while in (Huang et al., 2016) entire blocks of layers were randomly dropped during training. However, the first paper which, to our knowledge, really investigated neural networks on random geometries was the pioneering work of (Xie et al., 2019).

This paper proposed a concrete construction of a neural network based on a set of underlying graphs (one for each resolution stage of the network). Several models based on classical random graph generators were evaluated on the ImageNet dataset, achieving competitive results to the models obtained by NAS or hand-engineered approaches. Using the same mapping, very recently (Roberts et al., 2019) investigated neural networks based on the connectomics of the mouse visual cortex and the biological neural network of C.Elegans, obtaining high accuracies on the MNIST and FashionMNIST datasets.

Let us emphasize the key differences with the previous work. Firstly, in (Xie et al., 2019) there were separate random graphs for each stage of the neural network which dealt with a specific spatial resolution. In our case, we have a random graph for the whole network and dimensionality reduction is performed on a graph edge when necessary. Moreover, our network node is of a residual type as described in detail in section 3. Secondly, we introduced a general method of transforming a graph into a DAG which automatically takes into account the graph structure. Thirdly, we introduced a novel method of directly generating random DAGs as well as using graphs derived from fMRI networks. In fact, most of our best networks belonged to these new families. Finally, our focus was on a detailed study of numerical graph characteristics in relation to the associated neural network performance.

3. From a Directed Acyclic Graph to a Neural Network

In order to transform a directed acyclic graph to a neural network, we use a mapping similar to (Xie et al., 2019). The edges of the graph represent the flow of the information in the network and the nodes correspond to the operations performed on the data. For each node, the input from the ingoing edges is firstly aggregated using a weighted sum. Next, a ReLU Conv2d Batch-Norm block is applied. Finally, in addition to the procedure in (Xie et al., 2019), we introduce a residual connection from the aggregated signal to the output of the triplet block. The residual connection always performs a projection (implemented by a \(1 \times 1\) convolution, similar to ResNet C-type connections (He et al., 2016)). The result of this procedure is then propagated independently by each outgoing edge (see Figure 1). The only node that does not follow this construction is the output node, which performs a global average pooling on the weighted sum of its inputs and then applies a dense layer with the number of output neurons equal to the target dimension.

In the task of image recognition, typical neural network architectures usually perform a reduction of the spatial resolution of the feature maps with a simultaneous increase in the number of channels. A set of connected layers operating in the same resolution is referred to as a stage. We divide the network architecture obtained from a DAG into 3 stages, denoted by different colours in the figures. The first stage operates on the original input resolution, with the number of channels \(C\) being set in the first (input) node of the graph. The subsequent stages operate on a decreased input resolution and increased number of output channels by a factor of 2, with respect to the previous stage. In order to perform the downsampling, on every edge that crosses the stages we execute the same block of operations as in a standard node, but use convolutions with stride 2. Contrary to (Xie et al., 2019), we allow for multiple edges to connect different stages, instead of sampling stages as separate DAGs and connecting them with one single edge. Note that we also allow for hops - edges that directly connect the first stage with the last, performing a reduction by factor 4.

4. The Space of Random Graphs and DAGs

We performed a massive empirical study of over 1000 neural network architectures based on 5 graph families and 2 auxiliary constructions (see Fig. 2). We summarize below their main characteristics.

Erdős-Rényi (er) In this model, given a parameter \(p \in [0, 1]\), each possible (undirected) edge arises independently of all the other edges with probability \(p\) (Erdős & Rényi, 1960).

Barabási-Albert (ba) The Barabási-Albert model favors the formation of hubs, as the few nodes with high degree are more likely to get even more connections in each iteration. Therefore graphs produced by this model are associated with scale-free networks. Apart from the number of nodes these graphs have a single integer parameter (Barabási & Albert, 1999).
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Figure 2. The UMAP embedding of the space of neural networks analyzed in the present paper, obtained from the dataset of the corresponding graph features mentioned in section 5.4. Different colors represent different graph families. The central blob includes graphs with $n = 60$ nodes.

**Watts-Strogatz (ws)** - The graphs obtained by this method tend to have the small-world property. There are two non-trivial parameters: an integer and a real probability (Watts & Strogatz, 1998).

**Random-DAG (rdag)** - The models mentioned so far produce undirected graphs, which need to be later transformed to DAGs. To overcome this drawback, we propose a new algorithm that directly constructs a random DAG. This procedure and its parameters is thoroughly explained in section 4.2.

**fMRI based (fmri)** - In addition to the above algorithmic generators we also introduce a family of graphs that are based on resting state functional MRI data from the Human Connectome Project. The exact method used to derive DAGs from the fMRI partial correlation matrices is described in detail in section 4.3. Apart from the number of nodes, this family has a single thresholding parameter.

Moreover, we considered two auxiliary types of graphs:

**Bottleneck graphs (bottleneck)** - For some graphs from the above families, we introduced a bottleneck between the various resolution stages (see section 5.1).

**Composite graphs (composite)** - We obtained these graphs by maximizing

$$
\left( \frac{\log \text{num\_paths}}{\text{num\_nodes}} \right)^{\frac{1}{2}} - 2\text{grc} - \text{avg\_clustering} \quad (1)
$$

where grc is the global reaching centrality of the graph.

For each of the above families we fix a set of representative parameters\(^1\). Then for every family-parameters pair we sample 5 versions of the model by passing different random seeds to the generator. Using this procedure we create 475 networks with 30 nodes and 545 networks with 60 nodes. We train all networks for 100 epochs with the same settings on the CIFAR-10 dataset\(^2\). For each network we set the number of initial channels $C$ in order to obtain approximately the same number of parameters as in ResNet-56 (853k).

Figure 3. The gray nodes (orphan nodes) in the DAG either do not have an input from previous stages of processing or do not have an output. Hence we add the red edges from the immediately preceding node or to the immediately succeeding node.

### 4.1. From a Graph to a Directed Acyclic Graph

Within the framework of the present paper, where we consider standard neural networks with no recurrent connections, we need to deal with a directed acyclic graph (DAG). Yet, the vast majority of families of random graphs involve undirected graphs and so do not fall into this category. Therefore, we need a general procedure for picking the directionality of each edge. This can be achieved by picking a total ordering of the nodes of the graph (e.g. by labeling the nodes by integers) and setting the directionality of an edge from the lower to the higher node number. The key point is, of course, the precise method how to introduce the global ordering of the nodes.

The paper (Xie et al., 2019) used either a random assignment of integers to the nodes, or a process which was tied to a specific random graph construction procedure. Here we propose a general method, agnostic about the graph construction process, which automatically incorporates some knowledge about the graph structure. In particular, we would like the adopted directionality structure to be intuitively most economical and natural for the given graph.

To this end, we start with a 2D graph embedding, which is well suited for visualization. This could be e.g. Fruchterman-Reingold (Fruchterman & Reingold, 1991)\(^3\). Refer to Supplementary Materials F for a full list. We provide a full description of the training procedure in Supplementary Materials A. As a cross-check we also computed the performance for a majority of networks with 60 nodes (excluding bottleneck ablations) on CIFAR-100 (see section 5.2), using the same training regime.
or Kamada-Kawai (Kamada & Kawai, 1989) embedding. In our simulations we adopted the latter. The advantage of this embedding is that the spatial structure (i.e. node coordinates) is coupled to the abstract internal connectivity structure of the graph so that the total spring energy associated to the edge lengths is minimal.

We fix the ordering by sorting the nodes by the $x$-coordinate of the Kamada-Kawai embedding and orient the edges accordingly. However, in order to put a neural network on a DAG, we need to have only a single input node and a single output node. Moreover, all paths on the DAG should arise from paths going all the way from the input to the output node. Hence we need to fix some orphan nodes like the ones in Fig. 3, by adding a connection from the node with the preceding number or adding a connection to the node with the succeeding number.

Algorithm 1 Random DAG 

Input: nodes $i = 0, \ldots, N − 1$, 
number of outgoing edges $n_i^{\text{out}}$, 
size of a local neighbourhood $B$, 
real $\alpha$, function $f(x)$

for $i = 0$ to $N − 2$ do
    if node $i + 1$ does not have an ingoing connection then
        make an edge $i \rightarrow i + 1$
    end if
    while not all $n_i^{\text{out}}$ outgoing edges choosen do
        Make randomly the edge $i \rightarrow j$ with the weight
        
        \[w_{ij} = (n_j^{\text{out}})^\alpha f\left(\left\lfloor \frac{j - i}{B} \right\rfloor\right)\]
        provided $j > i$ and $i \rightarrow j$ does not exist so far
    end while
end for

4.2. Direct Construction of Random DAGs

As the mapping from an undirected graph with cycles into a DAG can seem as somewhat artificial, it is interesting to develop a method of directly generating random DAGs, which would be flexible enough to generate various qualitatively different kinds of graph behaviours.

We present our method in Algorithm 1. We start with $N$ nodes, with a prescribed ordering given by integers $0, \ldots, N − 1$. For each node $i$, we fix the number of outgoing edges $n_i^{\text{out}}$ (clearly $n_i^{\text{out}} < N − i$). Here we have various choices leading to qualitively different graphs. E.g. sampling $n_i^{\text{out}}$ from a Gaussian (or setting $n_i^{\text{out}}$ to a constant) would yield approximately homogeneous graphs. Taking a long tailed distribution like Laplace, would yield some outgoing hubs. One could also put in the large outgoing hubs by hand in a background of constant and small $n_i^{\text{out}}$.

For each node $i$ we then randomly choose (with weight $w_{ij}$ given in Algorithm 1) nodes $j > i$ to saturate the required $n_i^{\text{out}}$ connections. The freedom in the choice of weight gives us the flexibility of preferential attachment (through the parameter $\alpha$) and/or imposing local/semi-local structure. Since we do not want the integer ordering to be really just a 1d coordinate, we define a local neighbourhood size $B$ so that differences of node labels of order $B$ would not matter. In the simulations we set $B = 5$ or 10. This motivates the form of function $f(x)$:

\[f(x) \equiv f\left(\left\lfloor \frac{j - i}{B} \right\rfloor\right)\]  

where $\lfloor a \rfloor$ denotes the floor of $a$. Different choices of $f(x)$ lead to different connectivity structures of the DAG. An exponential $f(x) = \exp(-Cx)$ leads to short-range connections and local connectivity. The power law scaling $f(x) = 1/x$ leads to occasional longer range connections, while $f(x) = 1$ does not lead to any spatial structure at all. In this work, we investigated the above three possibilities.

4.3. Graphs Associated with fMRI Networks

In this paper we decided to supplant the families of algorithmically generated random graphs by including a family of graphs derived from resting state connectome from fMRI data. We used the network connectomes provided by the Human Connectome Project (Van Essen et al., 2013) based on resting state fMRI data of 1003 subjects (Smith et al., 2013). As an input for graph construction, we used the released (z-score transformed) partial correlation matrix for 50- and 100-component spatial group-ICA parcellation.

In order to obtain a 30- or 60- node graph, we took the absolute value of the entries of the partial correlation matrix (of the 50- and 100- component version respectively), used a range of thresholds\(^4\) to binarize the matrix which was then interpreted as an adjacency matrix of a graph. Since a priori the graph obtained in this way does not need to be connected, we took the largest connected component. Here typically the node number was still larger than the target 30 or 60, so we used Induced Subgraph Random Walk Sampling algorithm\(^5\) to subsample the graphs to the required number of nodes. Since the subsampling is stochastic, the choice of random seed produces the 5 differing versions of the fMRI graph\(^6\).

Let us emphasize that one should not treat the fMRI graphs (and especially the corresponding neural networks) as pro-

\(^4\)From 2.0 to 5.0 (or 4.9) for the 50-component case in 0.5 steps.
\(^5\)From github.com/Ashish7129/Graph_Sampling.
\(^6\)At highest threshold which required the mildest subsampling, these versions did not differ much.
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Providing a realistic model of how the human brain processes information in such a visual classification task. The latter process occurs of course on a much smaller scale than the brain-wide networks. Also we did not attempt to estimate in any way the directionality of the edges, as in any case our approach requires ultimately a directed acyclic graph. The interest in using these data is that it nevertheless encodes some global features of information processing by the brain. Moreover, these graphs are not produced by a standard mathematical graph generating algorithm, so they bring more variety to the range of considered networks.

Figure 4. Original graph (left) and its bottleneck variant (right).

Figure 5. The CIFAR-10 test accuracy for selected pairs of networks and their bottleneck \((b)\) prefix ablations. From left: best \(\text{rdag}\) with 30 nodes, best \(\text{rdag}\) with 60 nodes, maximally connected DAG \((\text{er}\) with \(p = 1.0)\) on 30 and 60 nodes.

5. Key Results

In this section we discuss the most interesting results obtained in our research.

5.1. The Effect of Bottlenecks

As noted in section 2, one difference between the networks of (Xie et al., 2019) and our construction was that in the former case, there were separate random graphs for each processing stage of a specific resolution, which were connected with a single gateway. In our case we have a single graph which encompasses all resolutions.

In order to check whether such a single gateway between different resolutions could be beneficial or not, for a set of graphs we artificially introduced such a bottleneck by first erasing all but one inter-resolution edges (this is illustrated in Fig. 4) and then fixing possible orphans as in Fig. 3.

We found that, systematically, the introduction of a bottleneck deteriorates performance (see Fig. 5). Hence multiple resolution reduction pathways are beneficial.

Figure 6. The CIFAR-10 (y-axis) and CIFAR-100 (x-axis) test accuracies. Each datapoint contains results averaged over the versions of the models. The Pearson correlation coefficient for this data is equal to 0.821.

5.2. CIFAR-10 versus CIFAR-100 Consistency

In addition to the CIFAR-10 task, we trained all networks with 60 nodes (except for the bottleneck ablations) on the CIFAR-100 dataset. The motivation for this experiment was to verify whether the graph families which performed best in the first problem achieve also high results in the second. Indeed, we observe a significant correlation 0.821 (see Fig. 6) between the respective test accuracies (averaged over the 5 random realizations of each graph type). Especially noteworthy is the consistency between the groups of best and worst graphs for the two datasets.

5.3. Long- vs. Short-range Connections

The algorithm for directly generating random DAGs allows for modifying, in a controllable way, the pattern of long- versus short-range connectivity. This is achieved by changing the function \(f(x)\) from an exponential, leading to local connections, through a power law, which allows for occasional long range connections, to a constant function, which does not impose any spatial order and allows connections at all scales. The results are denoted in Fig. 7. We observe, that within this class of networks, the best performance comes from networks with primarily short range connections and deteriorates with increasing length.

This may at first glance seem counter-intuitive, as skip connections are typically considered as beneficial. However,
Figure 7. The CIFAR-10 test accuracy averaged over different versions (random seeds) of random DAG models with 30 nodes and constant number (2-5) of output edges \( n_{out} \). The symbol \( \text{exp3} \) stands for exponential weighting function \( f(x) \), \( \text{pow1} \) for a power law and \( \text{one} \) for a constant.

Figure 8. The test accuracy versus selected network features. We indicate the best (equal or above 93.25%) models as orange, the worst (below 92%) as green, and the rest as blue. For more details and data processing refer to Supplementary Materials C.

the effect of long range connections which is associated with easier gradient propagation is already taken care of by the residual structure of each node in our neural networks (see section 3). One can understand the deterioration of the network performance with the introduction of long term connections as coming from an inconsistency of the network with the natural hierarchical semantic structure of images. This result leads also to some caution in relation to physical intuition from critical systems where all kinds of power law properties abound.

5.4. The Partial Failure of Classical Graph Invariants

One of the key motivations for this work was to understand what features of the underlying graph are correlated with the test performance of the corresponding neural network. To this end, for the analysis we used 54 graph features, mostly provided by the networkx library (for a full list see Supplementary Materials C) as well as some simple natural ones, like the logarithm of the total number of paths between the input and output or the relative number of connections between stages with various resolutions.

It turns out that none of the classical features by itself is enough to isolate the best performing networks. The worst networks are, however, to a certain extent extreme and can be more or less identified (see Fig. 8 for a representative example and more plots in the Supplementary Materials E).

We analyzed various ML regressors (for predicting test accuracy of the given graph type) or classifiers (for predicting the best performing networks) as well as feature selection procedures. See Fig. 10 for the results for a Random Forest regressor. The Random Forest nicely selects a class of best performing graphs, however the complexity of the model makes it difficult to interpret. Therefore, in the following, we will introduce new numerical characteristics which will pick out a range of well performing graphs.

5.5. The Worst Networks

As mentioned before, several investigated network features seem to be able to discriminate the worst networks (Fig. 8). Those networks are usually characterized by long distances between any two nodes in the graph, resulting in long chains of operations and sparse connections. An example of such a graph is presented in Fig. 11. In addition, we verified that purely sequential 1d chain graphs (node \( i \) is connected only to node \( i+1 \)) gave indeed the worst performance.

5.6. The Best Networks – quasi-1d Graphs

We observed that the best networks for the 60 node (see Table 1) and 30 node graphs belong predominantly to the Random DAG category with short range connections (i.e. exponential \( f(x) \)). One generic visual feature of these graphs is their quasi-1d structure (see the first two graphs in Fig. 9). There is a definite global ordering in the feed-forward processing sequence defining the 1d structure, yet locally there are lots of interconnections which most probably implement rich expressiveness of feature representations. These models have a very large number of paths between the input and the output. This is, however, not a defining feature, as maximally connected DAGs with maximal possible number of paths do not fall into this category and have worse performance (recall Fig. 5). Intuitively such an architecture is somewhat similar to DenseNets (Huang et al., 2017), although without bottlenecks. In contrast, filament-like almost 1d models like some Watts-Strogatz networks (see e.g. Fig. 11) have in fact significantly worse performance.

We would like now to characterize these graphs purely in terms of some numerical graph features without recourse to their method of construction. This is not \textit{a priori} a trivial task. On the one hand, one has to be sensitive to the quasi-1d structure, on the other hand the filament-like almost 1d models like some Watts-Strogatz networks (see e.g. Fig. 11) have in fact significantly worse performance.

Note that these are results for a single simulation with specific initialization. We may of course expect differences with other initializations. The key point of Table 1, however, is the predominance of specific types of graphs appearing in the top-10.
graphs are quite similar in this respect, yet they yield very bad performance. So numerical graph invariants which are positively correlated with the 1-dimensionality tend to have similar or even larger values for the very bad graphs.

A condition which would eliminate the unwanted latter graphs is $n_{\text{bottlenecks}} = 0$, where a bottleneck edge is now defined more generally by the property that cutting that edge would split the graph into two connected components. The easiest way now to numerically encode the quasi-1d character is to use the Kamada-Kawai embedding, perform PCA on the set of node coordinates and require sufficiently anisotropic explained variance ratio. Hence we define\(^8\)

$$\text{pca}_{\text{elongation}} = 2 \cdot (\text{variance}_{\text{ratio}}[0] - 0.5) \quad (3)$$

It turns out that requiring

$$\text{pca}_{\text{elongation}} > 0.25 \quad \text{and} \quad n_{\text{bottlenecks}} = 0 \quad (4)$$

is already quite a good condition giving 102 networks (83 rdag, 14 ws and 5 fmri) with accuracy $92.96 \pm 0.26$ for 60 node networks\(^9\). This includes 7 out of the 10 best networks from Table 1. One could try to refine this further

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\(^8\)Note however, that despite appearances this is a quite complex invariant of the original abstract graph, as the Kamada-Kawai embedding depends on the whole global adjacency structure through the spring energy minimization. Hence the nature of the embedding encodes nontrivial relevant information about the graph.

\(^9\)For 30-node networks one would get 97 networks with $92.87 \pm 0.29$. Therefore it is better to increase the threshold to say 0.5 which would yield 42 with $92.99 \pm 0.24$ (and 67 networks with accuracy $92.98 \pm 0.25$ for 60 node networks).
Table 1. The best 10 networks with 60 nodes. Q1D denotes the criterion (4).

| Network                  | Accuracy | Q1D |
|-------------------------|----------|-----|
| RDAG_CONSTANT_5_60_v3   | 93.61    | ✓   |
| RDAG_CONSTANT_3_B10_EXP3_60_v3 | 93.58    | ✓   |
| RDAG_CONSTANT_3_B10_EXP3_60_v4 | 93.49    | ✓   |
| FMRI_50_60_v0           | 93.45    | ×   |
| RDAG_CONSTANT_3_B10_60_v4 | 93.35    | ✓   |
| RDAG_CONSTANT_2_B10_EXP3_60_v0 | 93.34    | ✓   |
| RDAG_CONSTANT_2_B10_EXP3_60_v2 | 93.34    | ✓   |
| WSKX_60_60_6_v1         | 93.33    | ×   |
| RDAG_CONSTANT_4_60_v3   | 93.33    | ✓   |
| FMRI_40_60_v0           | 93.32    | ×   |

using other features which would be sensitive to long range connections, but here we were aiming at the simplest possible (and interpretable) numerical characterization of the good quasi-1d graphs.

Let us also mention that there are some qualitatively different networks (see e.g. the fmri network in Fig. 9) in the fmri class as well as the ba class which have quite good performance, although generically worse than the quasi-1d case (see Fig. 6). It seems, however, quite difficult to identify a numerical characterization which would pick out the best networks from this category (see e.g. Fig. 10 for the range of random forest predictions below 92.75). Indeed, there are also some individual highly ranked ws networks, which have rather badly performing counterparts with the same ws generator parameters and differing only in the random seed.

6. Summary and Outlook

We have performed an extensive study of the performance of artificial neural networks based on random graphs of various types, keeping the training protocol fixed. The number of parameters for each network was approximately fixed to be equal to the number of parameters of a ResNet-56 network for CIFAR-10.

Apart from the classical families of random graphs (Erdős-Rényi, Barábasi-Albert and Watts-Strogatz), we introduced an algorithm for directly generating random directed acyclic graphs (rdag), which is very flexible and can be tuned to generate DAGs of various types. In particular, it is well suited for modifying short- and long-range connectivity. In addition, we constructed a family of graphs based on resting state fMRI connectivity networks of the human brain. Another contribution of the present paper was to introduce a general procedure of going from a graph to a directed acyclic graph (which takes into account the structure of the graph) necessary for a feed-forward neural network.

A class of networks which had the best performance in our simulations (clearly better than the reference ResNet-56 network) were networks which could be characterized as quasi-1-dimensional, having mostly local connections with a definite 1-dimensional hierarchy in data processing (one can dub this structure as local chaos and global order). These were predominantly networks in the rdag family. We also introduced a very compact numerical characterization of such graphs.

It is worth noting, that some of the fmri based graphs were also among the best performing ones (together with some ws and ba ones). However, for the moment we lack a clear cut numerical characterization of these “good” graphs as there exist graphs with apparently similar structure and numerical invariants but much worse performance.

Among other structural observations made in this paper, we noted that long range connections were predominantly negatively impacting network performance. Similarly, artificially imposing a bottleneck between the processing stages of various resolutions also caused the results to deteriorate.

We believe that the performed research will open up space for numerous further investigations. The massive dataset could be used for independent further exploration of the interrelation of graph topology and network performance. The best and worst performing classes of networks identified here may be used to focus further research in specific directions.

We expect that once we move to a greater number of nodes, we may see much more marked differences between the various network types, as the main random graph families are really defined asymptotically and for a small number of nodes may tend to blend between themselves for some choices of parameters. Considering larger graphs would be especially interesting in view of the flexibility of the random DAG algorithm introduced in this paper, which allows to generate a wide variety of networks, of which we studied only a subset here.

Another interesting direction of research is the modification of the precise network counterparts of the graph nodes. In this paper we adopted to some extent the formulation of (Xie et al., 2019), but there is definitely room for significant changes in this respect.

Finally, let us note that apart from any practical applications in the search for better network architectures, the results on the neural network performance as a function of graph architecture should yield a lot of data which could contribute to the theoretical quest for the understanding of the efficacy of deep learning.

10The graph architectures, the test accuracies as well as the PyTorch code will be available on github: [https://github.com/rmldj/random-graph-nn-paper](https://github.com/rmldj/random-graph-nn-paper)
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A. Training Regime

All the networks are trained for 100 epochs on the CIFAR-10 dataset with the standard train-test split. All models are optimized using the SGD algorithm with batch size 128, initial learning rate 0.1 and momentum 0.9. In addition, we use a weight decay equal to 1e–4. The learning rate is decreased to 0.01 and 0.001 in the 80th and 90th epoch respectively. This setting is the same as the one used in ResNet, the only exception is that we train for less epochs and therefore perform the learning rate drop earlier. The number of the initial channels $C$, which characterizes the size of the model, is set for each network separately, so that the total number of parameters is approximately the same as in the ResNet-56 model for CIFAR-10 (853k). For the experiment on CIFAR-100 in section 5, we use the same setting as above and perform the train and evaluation on the standard train and test split.

The code for the experiments was prepared in the python programming language, with the use of pytorch and networkx packages. For the ResNet model we use the implementation provided by Yerlan Idelbayev in https://github.com/akamaster/pytorch_resnet_cifar10. The training of neural network models was conducted on GeFroce RTX 2080 Ti and GeForce GTX 980 graphic cards. The mean time of one epoch was 56.12s ($\pm 26.59$).

B. Comparison of Graph Node Orderings

In this section we investigate the performance of a neural network in relation to the node ordering provided in the DAG transformation procedure. We fix the underling undirected graph to a $\epsilon r$ network with parameters $n = 30$ and $p = 0.2$. For both the Fruchterman-Reingold and Kamada-Kawai embeddings, we consider four methods for obtaining the ordering of the nodes based on their coordinates:

- **x-coordinate** ($x$) - The ordering is given by the x-coordinate of the nodes.
- **radial** ($r$) - The ordering is given by the norm of the coordinates.
- **reversed radial** ($rr$) - The reversed version of the radial ordering.
- **bifocal** ($bf$) - First, two nodes with the largest minimum distance are selected. These nodes will be the output and input nodes of the network. The rest of the nodes are ordered by $d_i = \frac{d_{i,1} - d_{i,2}}{d_{i,1} + d_{i,2}}$, where $d_{i,1}$, $d_{i,2}$, are the distances from node $i$ to the chosen input and output nodes.

The impact of those orderings on the flow of the resulting DAG is presented in Fig. 12. The performance of the corresponding neural network models is presented in Fig. 13. We choose the Kamada-Kawai embedding with the x-coordinate method for the rest of the experiments, as it provides good mean results, at the same time having low standard deviation.

![Figure 12](image-url)  
*Figure 12. The visualisation of different graph orderings on the Kamada-Kawai embedding.*

![Figure 13](image-url)  
*Figure 13. The test accuracy on CIFAR-10 dataset on the $\epsilon r$ graph with 30 nodes and $p = 0.2$ averaged over the versions of the model. The 'FR' and 'K' prefixes stand for the two tested graph embeddings (Fruchterman-Reingold and Kamada-Kawai). For each of the embeddings four node orderings are investigated: x-coordinate, radial, reversed radial and bifocal. The orderings are denoted in the suffix of the label respectively as $x$, $r$, $rr$ and $bf$.*
C. Collecting and Processing Graph Features

For each DAG network we computed 54 features. All attributes are rescaled using the min-max scaling. Selected features are also raised either to the power 1/2 or 1/4. For the summary, please refer to Table 4.

D. Evaluating Various Regression Models

We divide the dataset of graph attributes for networks with 60 nodes into train and test sets, having respectively 300 and 245 samples. Note that we do not allow for separate versions of the same graph model to appear both in test and train dataset. As the dependant variable we select the test accuracy on CIFAR-10 dataset averaged over different versions of the model. We investigate six different regression methods: Support Vector Regression (SVR), K-Nearest Neighbors (KNN), Random Forest Regressor (RF), AdaBoost (AB), Gradient Boosting Regressor (GBR) and Linear Regression (LR) with ridge, lasso and combined (Elastic Net model) regularization.\(^\text{11}\) For each of them we select the best hyper-paramters setting by performing a 5-fold cross-validation and picking the model with the lowest mean squared error averaged over the folds. Next, we evaluate the models on the test dataset. The results are presented in Table 2. For the list of considered hyper-parameters please refer to Table 3.

\(^{11}\)We use the implementations provided in scikit-learn package.

\begin{table}[h]
\centering
\begin{tabular}{lcc}
\hline
\textbf{MODEL} & \textbf{PARAMETER} & \textbf{VALUES} \\
\hline
SVR & C & [0.001, 0.01, 0.1, 1.0, 10.0, 100.0] \\
& gamma & ['scale', 'auto'] \\
KNN & n_neighbors & [3, 5, 7, 11] \\
& weight & ['uniform', 'distance'] \\
& leaf_size & [5, 15, 30, 45, 60] \\
& p & [1, 2] \\
RF & n_estimators & [10, 50, 100] \\
& max_depth & [1, 3, 5, 7, 15, 30] \\
AB & base_estimator & [DT, SVR, KNN] \\
& learning_rate & [0.001, 0.01, 0.1, 1.0] \\
& loss & ['linear', 'square', 'exponential'] \\
GBR & n_estimators & [10, 50, 100] \\
& learning_rate & [0.1, 0.01, 0.001] \\
& loss & ['ls', 'huber'] \\
& max_depth & [1, 3, 5, 7, 15, 30] \\
LR-RIDGE & alpha & [0.001, 0.01, 0.1, 1.0, 10, 100] \\
LR-LASSO & alpha & [0.001, 0.01, 0.1, 1.0, 10, 100] \\
LR-ELASTIC-NET & alpha & [0.001, 0.01, 0.1, 1.0, 10, 100] \\
& l1_ratio & [0.25, 0.5, 0.75] \\
\hline
\end{tabular}
\caption{The considered hyper-parameters for each model. 'DT' in AdaBoost states for Decision Tree. For the parameters names we use the same convention as the scikit-learn package.}
\end{table}

E. CIFAR-10 Test Accuracy versus Graph Attributes

For every investigated graph attribute we plot the test accuracy on CIFAR-10 dataset versus the value of the attribute (after the processing described in section C). The results are presented in Fig. 14.

F. Summary of the Investigated Graph Families

In total, we have analyzed 1020 graphs: 475 with 30 nodes and 545 with 60 nodes. The number of models in each graph family, as well as the investigated graph generator parameters are given in Table 5.
Table 4. The list of computed graph features together with their definitions. The last column indicates whether an additional transformation (raising to the power 1/2 or 1/4) was applied after the rescaling. An asterisk (*) after the feature name indicates that it was computed with the `networkx` package (see https://networkx.github.io/documentation/stable/reference/ for documentation).

| Feature Name                  | Definition                                                                 | P  |
|-------------------------------|---------------------------------------------------------------------------|----|
| 1. DEGREE ASSORTATIVITY*      | assortativity of the graph by degree                                      | –  |
| 2. MAX DEGREE                 | maximum degree in the graph                                               | 1/2|
| 3. MEAN IN DEGREE             | mean indegree                                                            | 1/4|
| 4. MEAN OUT DEGREE            | mean outdegree                                                            | 1/2|
| 5. MIN DEGREE                 | minimum degree                                                            | 1/4|
| 6. OUTER EDGES                | relative number of the edges connecting different stages                 | –  |
| 7. NUM NODES                  | number of nodes                                                           | –  |
| 8. NUM EDGES                  | number of edges                                                           | 1/2|
| 9. REDUCE FRAC                | number of reduce edges divided by all nodes                               | –  |
| 10. EDGES PER NODE            | number of edges divided by the number of nodes                            | 1/2|
| 11. DENSITY*                  | density of the graph                                                      | 1/2|
| 12. TRANSITIVITY*             | number of triangles divided by all triangles                              | 1/2|
| 13. AVERAGE CLUSTERING*       | average clustering coefficient of the nodes                               | 1/2|
| 14. AVERAGE NODE CONNECTIVITY*| average local node connectivity                                           | 1/4|
| 15. AVERAGE SHORTEST PATH LENGTH| average length of all pairs of shortest paths                             | 1/4|
| 16. S METRIC NORM*            | normalized sum of the product of nodes degrees for each edge             | 1/2|
| 17. GLOBAL REACHING CENTRALITY*| global reaching centrality of the graph                                  | 1/2|
| 18. EDGE CONNECTIVITY*        | local edge connectivity between the input and output node                 | 1/4|
| 19. MODULARITY TRACE*         | sum of eigenvalues of the modularity spectrum                             | 1/2|
| 20. INTRASTAGE                | relative number of edges within stages                                    | –  |
| 21. INTERSTAGE                | relative number of edges crossing one stage                                | –  |
| 22. HOPS PER NODE             | relative number of edges crossing more than one stage                     | 1/4|
| 23. MEAN DEGREE               | mean node degree                                                          | 1/4|
| 24. STD DEGREE                | standard deviation of the node degree                                     | 1/4|
| 25. SPAN DEGREE               | maximum degree devided by minimum degree                                  | 1/4|
| 26. 021D*                     | number of 021D triads (computed by triadic census)                        | 1/2|
| 27. 021U*                     | number of 021U triads (computed by triadic census)                        | 1/2|
| 28. 021C*                     | number of 021C triads (computed by triadic census)                        | 1/2|
| 29. 030T*                     | number of 030T triads (computed by triadic census)                        | 1/4|
| 30. LOG PATHS                 | logarithm of the number of all paths from input to output                | 1/2|
| 31. MEAN PATH                 | mean path length from input to output                                     | 1/2|
| 32. STD PATHS                 | standard deviation of path lengths from input to output                   | –  |
| 33. MIN PATH                  | length of the shortest path from input to output                          | 1/4|
| 34. MAX PATH                  | length of the longest path from input to output                           | 1/4|
| 35. SPAN PATH                 | max path divided by min path                                              | 1/4|
| 36. CLOSENESS CENTRALITY*     | the reciprocal of the average shortest path distance to the output node  | 1/2|
| 37. CLOSENESS CENTRALITY MEAN*| mean of the closeness centrality for every edge                          | 1/2|
| 38. BETWEENNESS CENTRALITY MEAN*| mean of the relative number of all paths passing through given node     | 1/4|
| 39. CURRENT FLOW CLOSENESS CENTRALITY MEAN*| mean of the electrical-current model for closeness centrality              | –  |
| 40. CURRENT FLOW BETWEENNESS CENTRALITY MEAN*| mean of the electrical-current model for betweenness centrality         | 1/4|
| 41. SECOND ORDER CENTRALITY MEAN*| average second order centrality for each node                            | 1/2|
| 42. COMMunicability BETWEENNESS CENTRALITY MEAN*| average centrality based on communicability betweenness                  | 1/2|
| 43. COMMunicability START MEAN*| mean communicability of the input node                                   | 1/2|
| 44. COMMunicability END MEAN*  | mean communicability of the output node                                   | 1/2|
| 45. RADIUS*                   | radius of the graph                                                       | 1/2|
| 46. DIAMETER*                 | diameter of the graph                                                     | 1/4|
| 47. LOCAL EFFICIENCY*         | local efficiency of the graph                                              | –  |
| 48. GLOBAL EFFICIENCY*        | global efficiency of the graph                                             | 1/2|
| 49. EFFICIENCY*               | efficiency computed between the input and output nodes                    | 1/2|
| 50. PAGE RANK*                | page rank of the output node                                              | –  |
| 51. CONSTRAINT MEAN*          | average constraint of the nodes                                           | 1/2|
| 52. EFFECTIVE SIZE MEAN*      | average effective size of the nodes                                       | 1/2|
| 53. CLOSENESS VITALITY MEAN*  | average closeness vitality of the nodes                                   | –  |
| 54. WIENER INDEX*             | the normalized wiener index (sum of all pairs shortest distances)        | 1/2|
Figure 14. The test accuracy on CIFAR-10 dataset versus the investigated graph attributes. We indicate the best (equal or above 93.25%) models as orange, the worst (below 92%) as green, and the rest as blue. The shortcuts ’cc’, ’bc’ and ’comm’ stand for ’closeness centrality’, ’betweenness centrality’ and ’communicability’.
Table 5. The summary of analyzed graph families and their parameters.

| FAMILY    | TOTAL | GENERATOR PARAMETERS |
|-----------|-------|----------------------|
| ba        | 50    | Number of initially connected nodes $m \in \{2, 3, 5, 7, 11\}$. |
| bottleneck| 150   | Ablations on rdag graphs with constant $n_{out}$, on all composite and on all er with $p = 1.0$. |
| composite | 20    | Probability $p$ of the initial er graph: $p \in \{0.85, 0.99\}$. |
| er        | 75    | Probability $p \in \{0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0\}$. In addition, $p = 0.05$ for $n = 60$. |
| fmri      | 70    | Connectivity threshold $t \in \{2.0, 2.5, 3.0, 3.5, 4.0, 4.5\}$ for both 30- and 60-node graphs. In addition, $t = 4.9$ for 30 nodes and $t = 5.0$ for 60 nodes. |
| rdag      | 215   | For 30 nodes: $f(x) \in \{\exp(-2x), \exp(-3x), 1/x, 1\}$, for every constant $n_{out} \in \{2, 3, 4, 5\}$. In addition, one graph with $n_{out}$ sampled from Laplace distribution with scale 3 and two hub graphs. For 60 nodes: $f(x) \in \{\exp(-2x), \exp(-3x), 1/x\}$ for every constant $n_{out} \in \{2, 3, 4, 5\}$ and $B \in \{5, 10\}$. |
| ws        | 440   | Number of connections to the nearest neighbors in the initial ring $k \in \{2, 4, 6, 8\}$ for every rewiring probability $p \in \{0.0, 0.1, 0.2, 0.25, 0.3, 0.4, 0.5, 0.6, 0.75, 0.8, 1.0\}$. |
| **SUM**   | 1020  | |

Neural Networks on Random Graphs