Architecture Search by Estimation of Network Structure Distributions

Anton Muravev, Student Member, IEEE, Jenni Raitoharju, Member, IEEE, and Moncef Gabbouj, Fellow, IEEE

Abstract—The influence of deep learning is continuously expanding across different domains, and its new applications are ubiquitous. The question of neural network design thus increases in importance, as traditional empirical approaches are reaching their limits. Manual design of network architectures from scratch relies heavily on trial and error, while using existing pretrained models can introduce redundancies or vulnerabilities. Automated neural architecture design is able to overcome these problems, but the most successful algorithms operate on significantly constrained design spaces, assuming the target network to consist of identical repeating blocks. We propose a probabilistic representation of a neural network structure under the assumption of independence between layer types. The probability matrix (prototype) can describe general feedforward architectures and is equivalent to the population of models, while being simple to interpret and analyze. We construct an architecture search algorithm, inspired by the estimation of distribution algorithms, to take advantage of this representation. The probability matrix is tuned towards generating high-performance models by repeatedly sampling the architectures and evaluating the corresponding networks. Our algorithm is shown to discover models which are competitive with those produced by existing architecture search methods, both in accuracy and computational costs, despite the conceptual simplicity and the comparatively limited scope of achievable designs.

Index Terms—Automatic architecture design, deep learning, convolutional neural network, image classification.

I. INTRODUCTION

The recent successes of deep learning have attracted significant interest from theoretical and practical standpoints in numerous fields of knowledge [1]. Computer vision in particular has witnessed the development of multiple successful models, based on convolutional neural networks (CNNs), for tasks such as classification [2], [3], semantic segmentation [4], and detection [5]. Deep learning driven approaches have notably contributed to the fields of audio processing [6], bioinformatics [7], among other fields. While the growth of deep learning solutions over the years is impressive, their adoption brings many significant challenges. Some of these fall into the category of practical issues and have been the subject of extensive research. For example, the tendency of powerful models to overfit the training data is addressed by parameter regularization techniques, such as dropout [8], while the vanishing gradient problem is tackled by normalization [9], [10]. On the other hand, the theoretical foundation of deep learning is not yet comprehensively established, but receives growing attention, as optimality conditions are formulated [11], [12] and common techniques are explained [13]. The lack of interpretability of decisions made by deep models [14], [15] is a difficult problem to tackle, but has attracted increasing research attention recently [16]. Further concerns have been raised regarding secure practical use of deep models, as they were shown to be vulnerable to attacks utilizing malicious data [17].

One aspect of the neural networks, intricately tied to these challenges, is the architectural design: the choice of layer count, connection patterns, neuron operations, and their hyperparameters (convolution filter sizes, channel depth, etc.). It is well-known that some structural choices are associated with training difficulties; for example, depth increase causes the vanishing gradient problem [18]. Meanwhile, on a system level, the design guidelines of creating a deep network for a particular practical problem are not well established. The network design task thus becomes a time-demanding process, involving extensive trial and error. In practice, this issue is commonly avoided by using an already established pre-trained model of the same or related data domain as a feature extractor [19]. While effective, the latter approach presents problems of its own. Pre-trained models tend to be large and can lead to resource-consuming, largely redundant systems, whereas a much smaller network could have been sufficient. Specific features of the data may require specific layer types to be fully exploited [20]. Pre-trained models can carry over undesired biases from their original datasets [21]. Additionally, sharing the foundation means that such systems will naturally be more vulnerable to adversarial attacks. These problems can potentially be avoided by developing appropriate methods for automated task-specific network design.

The idea of automated neural network design dates back to the early 1990s [22]. The following decade saw a large volume of research on this problem, primarily focusing on evolutionary algorithms as solvers, both due to their gradient-free nature and shared biological inspirations [23]. This family of approaches would later be coined neuroevolution [24]. The research continued into the 2000s, with both improved evolutionary algorithms [24], [25] and other metaheuristic approaches, such as particle swarm optimization [25], as the search method. However, all of these algorithms share the need to perform many evaluations of the intermediate solutions, which, in the case of automated architecture design, requires training numerous candidate networks from scratch. Therefore, these approaches were computationally restricted to rather limited model complexity, and their practical applications remained primarily in control tasks and robotics, where these
The advent of deep learning, where training a single model can take days or weeks, caused manual design to once again become the primary approach. However, as architectural discoveries paved the way to models with a small number of parameters and superior performance [2], [8], the interest in automated design reemerged, taking advantage of both evolutionary optimization [28]–[31] and newer approaches, such as reinforcement learning [32]–[34]. The computational demand remains a major limitation and has hence been the focus of most recent works in the area [34]–[36].

Another concern is the growing semantic complexity of such algorithms. While they may yield successful architectures [31], their search behaviour is hard to analyze, which obscures the effects (whether positive or negative) of individual algorithmic steps and hinders comparisons. For instance, Zoph et al. [33] proposed a reduced search space: the network is represented as a repeating sequence of cells of a few types, where the internal structure of cells of the same type is identical and subject to optimization. Consequently, this design space has been adopted by a multitude of other approaches (see [31], [34], [37]), but the random search has recently been shown to be highly competitive as well, suggesting that previous successes may come from the expressivity of this space rather than algorithm specifics [38].

We propose a conceptually simple architecture search method, based on the estimation of distribution algorithms, specifically Population-Based Incremental Learning [39] and Univariate Marginal Distribution Algorithm [40]. We utilize a set of discrete probability distributions to describe the choice of layers in a feedforward deep network, assuming their independence. Together they form a network prototype, which is then iteratively updated by sampling and evaluating network models, until convergence is reached. The contributions of this paper can be summarized as follows:

- We propose a probabilistic representation of deep neural networks by expressing their structure as a set of layer type probabilities. A single prototype of the proposed form corresponds to not a single network, but a family of models, which can span the whole regions of the design space.
- We propose a CNN architecture search method based on the optimization of the above prototype, denoted Architecture Search by Estimation of network structure Distributions (ASED). As candidate networks are sampled and the individual probabilities converge to their extreme values, the algorithm naturally transitions from the global search to the local search, avoiding the suboptimal areas. The speed of convergence can be managed by additional proposed techniques.
- We experimentally demonstrate the comparable performance of our method to existing approaches in terms of both model performance and computational requirements, while using only feedforward structures without skip connections or explicit repeated motifs.

The rest of the paper is structured as follows. In Section 2, we review the related developments in the field of neural architecture optimization as well as elaborate on our inspirations. Section 3 describes our approach to architecture search. Section 4 contains the experimental results and their interpretations. Finally, Section 5 concludes the work and outlines potential future studies.

II. RELATED WORK

Ever since the wider adoption of multilayer perceptron structures ([41]), their architectures became subject to optimization. While general neural network design involved heuristic rules and empirical tests, a promising alternative was found in evolutionary optimization methods due to their ability to solve problems defined only by the target function, without requiring any gradient information [42]–[43]. Early works include [44]–[46]. However, all of these works shared common issues of prohibitive computational requirements and lack of robustness due to the highly noisy nature of the search space [23].

The small-scale neuroevolution reached a new peak when NEAT (NeuroEvolution of Augmented Topologies) [24] was introduced in 2002. The techniques that made NEAT differ from its predecessors are historical gene markings, allowing for straightforward and meaningful crossover, and speciation with fitness sharing, which allows promising individuals to more consistently reach their full potential. Despite the advantages and the flexibility it offered, NEAT remained limited to small-scale applications, such as control tasks with limited inputs (a problem which would later be tackled within reinforcement learning). Multiple subsequent variants of NEAT [25], [47], [48] aimed at efficient generation and representation of more complex networks with repeatable structural patterns. For example, HyperNEAT [25] did not encode network architectures directly, but rather as a set of neurons within a metric space, or substrate; a separate hypermodel called a Compositional Pattern-Producing Network (CPPN), given the metric coordinates of two neurons as input, outputs the connection weight between them, thus defining a structure. An evolved substrate variant of HyperNEAT, or es-HyperNEAT [48], avoided the need to explicitly define node geometry, allowing for discovery of a wider scope of structures. However, despite the greater representational expression of these methods, the overarching problems remained and the use was limited to specific small-scale applications [49].

The resurgence of interest for architecture optimization started in 2016, after the introduction of reinforcement learning driven Neural Architecture Search (NAS) in [32]. An LSTM-based recurrent neural network (a controller) is trained to output sequences of tokens, which decode to the parameter values of convolutional layers, such as filter size, count, and stride. The resulting neural network can be trained and evaluated. The controller can then be updated by the REINFORCE rule to maximize the expected accuracy of the generated networks. The major weakness of NAS is the computational cost of over 22000 GPU days on a standard CIFAR-10 image classification dataset. The follow-up work NAS-Net [33] represents the target network as a predefined sequence of repeating elements, known as cells. Each cell type shares the same internal structure, which is optimized in a graph form.
and can contain different convolution and pooling operations. During the search process, the total number of cells in the network is reduced to speed up computation, while the final discovered architecture is evaluated in a full-length sequence. Such a reduction of the design space has proven effective in guiding the search, thus boosting the accuracy and reducing the running time to 2000 GPU days, and has since been used in other works. Efficient NAS, or ENAS [33], achieved further speed-up (to less than 16 GPU hours) at the cost of some accuracy loss. It utilizes weight sharing, where the convolutional filter weights are identical between the cells and depend only on the position of the corresponding edge in the structural graph. Thus, training from scratch (which was necessary for the network evaluation) is no longer needed, and the tensor of shared weights can be finetuned via gradient updates in-between controller updates.

Evolutionary algorithms arose once again as a primary competitor to reinforcement learning based solutions. CoDeepNEAT [50] adapts the well-known NEAT procedure for deep networks by using two separate populations - blueprints and modules - for easier representation of repeating patterns. Genetic CNN [29] encodes layer connectivity in a population of binary strings and runs a standard genetic algorithm. Real et al. [29] run a distributed large-scale evolutionary process directly on the population of networks, where mutations can alter the network structure, parameters, or the training process. The following work of Real et al. [31] combines the evolutionary approach with the NAS-Net search space, surpassing reinforcement learning in anytime accuracy and setting a new state-of-the-art performance on the popular CIFAR-10 dataset, as well as generating comparatively simpler models. However, the computational cost remains extensive, clocking above 3000 GPU days. The similar approach is taken by the automatically evolving CNN (AE-CNN) [51], which runs a genetic algorithm on the population of networks composed of customized ResNet and DenseNet blocks, achieving competitive results.

While deep networks can be difficult for the neuroevolution to handle, a viable alternative can be found in expanding the operation set of the shallow networks, allowing for more powerful representations. Generalized Operational Perceptron (GOP) model substitutes the standard neuron by offering a wider choice of nodal and pooling operations instead of the standard multiplication and addition. The choice of operations can be optimized simultaneously with the network architecture by a greedy incremental procedure [52]. Operational Neural Networks (ONNs), composed of such units, have been shown to achieve superior performance to CNNs on some practical problems [33]. Most recently the heterogeneous GOP structures, where each layer can have neurons with differing operations, have received research attention [54]. While flexibility of operators allows ONNs to stay relatively shallow, it also results in a vast unstructured design space which is computationally costly to traverse.

Many recent works in architecture optimization utilize various techniques to reduce the computation needed, primarily by simplifying the evaluation procedure. SMASH [55] learns a hypernetwork that can predict weights for all the connections of an arbitrary deep network (given a specific representation), which reduces the need for training and makes random search a viable solution for discovering architectures. Progressive Neural Architecture Search (PNAS) [35] uses a separate recurrent network to approximately rank the candidate models without training them, allowing the search to focus only on more promising options. NASH [50] and LEMONADE [56] take advantage of network morphisms—operations that modify the structure of a trained network without affecting its output—to navigate the search space without training the models from scratch. Differentiable Architecture Search (DARTS) [37] provides a continuous relaxation of the NAS-Net cell structure problem and performs the search via gradient descent, iterating between the architecture and weight updates. While relatively more efficient in terms of computation, these methods do not address the issues of interpretability and semantic complexity.

There exists a number of works that model the network construction as a probabilistic process, sharing some similarities with the proposed approach. Methods based on reinforcement learning, such as NAS and its successors, use the probability of a given network to be produced from the current policy as a weight for the corresponding reward. InstaNAS [57] also has reinforcement learning at its core, but differs from other algorithms in this group, as it takes an instance-aware approach. Specifically, InstaNAS processes each data point by a separate network (a path within a large trained model), sampled from a parameterized distribution. NASBOT [58] models the architecture search as a Gaussian process. To facilitate this, the authors introduce a (pseudo)distance in the network design space and utilize an evolutionary algorithm as an optimizer. The most similar approach to ours is Probabilistic Neural Architecture Search (PARSENC) [59]. As in our work, PARSEC explicitly models a distribution to produce neural architectures of cells, including the assumption of independence between individual operations. However, this distribution operates on a level of NAS-Net cell, allowing PARSEC to take advantage of full weight sharing between the sampled model instances, while our method models the network as a whole. Moreover, the search procedure is different: PARSEC uses Monte Carlo empirical Bayes to iteratively update both the architectural priors and the tensor of shared weights, while we completely recompute the marginal probabilities over a subset of the samples and do not use weight sharing.

Our work draws inspiration from the estimation of distribution algorithms (EDAs) – the family of optimization methods originating from mid-1990s, which are closely related to genetic algorithms [60]. While most evolutionary algorithms maintain a candidate population, which implicitly defines the probability distribution of the solutions, EDAs define this distribution explicitly and tune its parameters throughout the optimization process. Our work mainly draws on two discrete univariate EDA, Population-Based Incremental Learning (PBIL) and Univariate Marginal Distribution Algorithm (UMDA) [40]. PBIL [39] generates an intermediate population via sampling, applies a selection procedure, and updates the probabilistic model in the direction of selected samples, using a learning rate parameter. UMDA [40] maintains the population of solutions, estimates a set of marginal probabilities from the best candidate(s) and uses them to produce the population
of the next generation. For more information on EDAs, their applications and recent developments, we direct the reader to the survey by Hauschild and Pelikan [61]. To the best of our knowledge, ours is the first work to explicitly apply the EDA formulation to the network architecture search problem.

III. METHODOLOGY

In this section, we describe and justify the proposed network representation, the design of the proposed algorithm Architecture Search by Estimation of network structure Distributions (ASED), as well as additional techniques to improve its capabilities.

A. Search Space and Network Representation

The problem of optimizing the structure of a neural network is extremely high-dimensional. The choice of layer types (convolution, pooling) alone produces a combinatorial problem that grows exponentially with the increase in depth, and that is without taking into account layer hyperparameters (filter size, stride, channel count) and weights. Connectivity patterns add another element of complexity, as structures such as skip connections and parallel branches have been found beneficial in manually designed models [8]. For this reason many recent architecture optimization algorithms, starting with NAS-Net by Zoph et al. [33], utilize a constrained search space based on repeated structural motifs. Instead of searching for the architecture of the entire network, they instead work with cells, which are small networks containing only a few layers. The target network is then constructed by repeating the cell a given number of times. This relaxation allows the cells to have almost arbitrary structures with the search remaining viable. Other advantage is the directly controllable trade-off between the network power and complexity by varying the number of cell repetitions. It is common to speed up the search by using less cells and then increase their number for the final evaluation of the discovered architecture. However, the natural drawback of this approach is the fact that only a small subset of network design space is reachable with such constraints, and potentially better architectures may not be discoverable. Therefore, we opt for optimizing the whole network simultaneously.

We model the deep neural network as a multivariate random variable coming from a known probability distribution. For the sake of tractability, we consider only the choices of layer types for optimization, resulting in the discrete distribution, while other hyperparameters are not directly tuned by the search procedure. Specifically, we bind the values of filter sizes and strides with the layer type choices and set the channel count to an externally defined constant for all the layers. We denote the set of possible layer types as \( L \) and call it the layer library. For the purpose of this work we choose to include the following ten common operations in the library:

- identity (output is equal to input),
- 1x1 convolution,
- 3x3 convolution,
- 5x5 convolution,
- 7x7 convolution,
- 3x3 dilated convolution (with dilation rate of 2),
- 5x5 dilated convolution (with dilation rate of 2),
- 2x2 max pooling,
- 3x3 max pooling (with stride 2),
- 3x3 average pooling (with stride 2).

We assume that the choice of each layer in the CNN is independently distributed. While this assumption is unlikely to hold in practice, it simplifies the formulation, and inter-layer interactions are implicitly taken into account during the search. Multivariate generalizations of the proposed method can potentially offer improvements, and are a promising future work direction. Given our assumption, a discrete distribution of network structures can be represented as a matrix of probabilities \( P \), where each row describes a layer and \( P_{ij} \in [0,1] \) is the probability of \( i \)-th layer being the \( j \)-th layer type from \( L \). Matrix \( P \) is henceforth called prototype. The dimensions of \( P \) are \( N \times |L| \), where \( N \) is the current number of layers in the network.

The probabilistic representation has a number of advantages over the population of networks. Matrices have a much wider range of available optimization approaches than graphs; many existing optimization algorithms outside of the scope of this work are straightforwardly applicable to the proposed representation. The prototype offers intuitive insight into the anytime state of the search, as the probability mass is always explicitly assigned for every point of the design space. The convergence of the search is easy to determine by how close the layer probabilities are to their extremes. Finally, the proposed representation can offer implementation advantages in distributed systems, as only a small prototype matrix needs to be transferred between computational nodes, rather than full-scale models.

The main drawback of the proposed representation is the fact that evaluating the prototype can only be done by sampling networks from it and training them from scratch. This is expected for architecture optimization, but, to minimize the sampling error, the number of samples has to be large, which can incur particularly high computational costs (especially for large values of \( N \)). While a number of techniques to minimize the evaluation costs exists, few of them are suitable for the prototype representation; for instance, due to the large variety of possible structures (of differing sizes), sharing the weights between them is not practical. Another drawback of the current formulation is its inability to represent networks with no strictly sequential dataflow, such as those featuring skip connections or branches. We consider the options to address this in the discussion of future work.

B. Search Algorithm

To construct an iterative architecture search algorithm with the above representation, three elements need to be defined - initialization, update and stopping condition. The proposed algorithm, denoted ASED, operates on a single prototype for the sake of simplicity. The depth of all networks on a given search step is the same due to the fixed prototype dimensions; to search across architectures of different sizes, we gradually increase the depth after each update step. While the prototype
rows are never removed, the inclusion of identity in our layer library means that, in practice, networks with less than \( N \) layers can be represented in \( N \) rows of the model, which is a starting layer count. While a more specific prior can be given, the uniform distribution is one that every network can be represented, which helps to emphasize early exploration. The choice of \( N \) should be carefully considered, as it is a small value that can result in premature convergence without sufficiently exploring the large portion of the design which case the prototype has converged to a single network is an indicator of the model to be "lost" unless an impractically large number of samples is evaluated (due to the curse of dimensionality).

To update the prototype, sampling of \( K \) candidate networks is performed first, with each layer sequentially selected from the discrete distribution given by the corresponding row of the prototype matrix. Each candidate model is then trained and evaluated on the target problem, and the temporary population is sorted by validation performance. The best \( K_s < K \) models are selected to directly induce the new prototype, which, due to the independence assumptions, takes the following form:

\[
P_{ij} = \frac{1}{K_s} \sum_{k=1}^{K_s} x_{kij},
\]

where \( x_{kij} \) is an indicator variable that is equal to 1 if \( k \)-th selected candidate network has \( j \)-th library item as \( i \)-th layer, and 0 otherwise. This update step is equivalent to the one used in the UMDA algorithm \( [40] \). Every update is followed by the addition of one or more rows to the prototype, according to the predefined schedule (denoted \( n(t) \)). These new layers are initialized with a uniform distribution. Note that we do not use elitism (explicitly preserving the best candidate between updates) as it can cause the bias towards initially discovered architectures to become too strong and promote premature convergence (recall that our approach gradually increases the problem dimensionality). The complete description of the ASED procedure is given in Algorithm 1. The search stops when the specified iteration limit \( t_{max} \) is reached or all the values of the prototype matrix become strictly 0 or 1, in which case the prototype has converged to a single network architecture.

\section{Avoiding Premature Convergence}

While the described search procedure navigates the search space by progressively narrowing down the region under consideration and should be capable of avoiding local minima, it can still get stuck in a local optimum and hence exhibit premature convergence. As the search progresses, individual layer probabilities tend to approach either 0 or 1 regardless of their immediate impact on the network performance, as is known from the theory of EDAs \( [62] \). The proposed algorithm does not allow for any mechanisms to limit this; in fact, such an effect is desirable for the search convergence. Moreover, once a probability has achieved the value of exactly 0 or 1, it becomes fixed and will not change thereafter, as all of the sampled networks will be the same with respect to the presence or the absence of the corresponding layer. The choice made is permanent, meaning that the dimensionality of the problem is essentially reduced from that point on. A subset of network structures becomes unreachable, which can be beneficial for navigating the design space, but can also mean the loss of potentially better solutions. We consider two different techniques to address this issue.

A common technique in EDAs involves capping the probabilities, such that extreme values are not achievable and each element instead spans the predefined range \([p_{min}, p_{max}]\), where \( p_{min} > 0, p_{max} < 1 \). In our setting, this means that there is always at least the probability of \( p_{min} \) for each layer to be selected in any position, removing irreversible choices. Probability capping is implemented by simple row-wise proportional normalization of the prototype matrix after every prototype update step. We adopt the approach where the upper cap \( p_{max} \) is explicitly given as a parameter and the lower cap is then computed as

\[
p_{min} = \frac{1 - p_{max}}{|L| - 1}.
\]

The normalization itself is then performed as follows:

\[
p_{ij}' = \begin{cases} p_{min} & \text{if } p_{ij} \leq p_{min} \\ p_{ij} \cdot m_i & \text{if } p_{ij} > p_{min} \end{cases},
\]

\[
m_i = \frac{\sum B_i + \sum S_i \cdot p_{min}}{\sum B_i},
\]

where \( S_i = \{p_{ij} | p_{ij} < p_{min}\} \) and \( B_i = \{p_{ij} | p_{ij} > p_{min}\} \) for \( i \in \{1, \ldots, N\} \).

\begin{algorithm}
  \caption{Architecture Search by Estimation of Network Structure Distribution (ASED)}
  \begin{algorithmic}[1]
    \State \textbf{Input:} \( L, N_{init}, t_{max}, K, K_s, n(t) \)
    \State \( N \leftarrow N_{init} \)
    \For {\( i \in \{1, \ldots, N_{init}\}, j \in \{1, \ldots, |L|\} \)}
      \State \( P_{ij} \leftarrow 1/|L| \)
    \EndFor
    \For {\( t \in \{1, \ldots, t_{max}\} \)}
      \State Sample \( K \) candidate networks from \( P \)
      \State Train and evaluate candidate networks
      \State Sort candidate networks by validation performance
      \State \( S \leftarrow K_s \) best performing candidate networks
      \State Recompute \( P \) based on \( S \) (Eq. 1)
      \State Add \( n(t) \) new rows to \( P \)
      \For {\( i \in \{N + 1, \ldots, N + n(t)\}, j \in \{1, \ldots, |L|\} \)}
        \State \( P_{ij} \leftarrow 1/|L| \)
      \EndFor
      \State \( N \leftarrow N + n(t) \)
      \If {\( \forall i, j \) \( P_{ij} \in \{0, 1\} \)}
        \State \textbf{break}
      \EndIf
    \EndFor
    \State \textbf{return} \( P \)
  \end{algorithmic}
\end{algorithm}
Another way to prevent the search from prematurely converging is to additionally modify the prototype between iterations. This can be done by applying a small random perturbation, similar to how the mutation is used in evolutionary algorithms. However, due to the search being driven by sampling, the effect of such mutation would be either insignificant or highly unpredictable. Instead, we opt for another operation, which we call prototype inversion, that replaces high probabilities with low values and vice versa. This prompts the search to explore exactly the previously discarded regions of the search space while the currently dominating choices become extremely unlikely (the latter aspect evokes similarities to the well-known tabu search, which is an optimization technique that explicitly forbids the reuse of already seen solutions [63]). Naturally, such an inversion operation is highly destructive and can prevent the search from progressing, so it needs to be executed only at some iterations of the algorithm. Additionally, we save the current prototype just before inverting it to make sure the information is not lost, which essentially means the ASED algorithm can produce multiple solutions before the stopping condition is met.

To establish an inversion condition, we need to find the measure of convergence, as performing the inversion too early and/or too often can hinder the search process. $L_2$-norm of the probability vectors is suitable for this purpose, as it spans the interval $[1/\sqrt{L}, 1]$. Here the lower bound corresponds to the uniform distribution and the upper bound is achievable only when a single element (layer type) takes value 1 with every other being 0. The $L_2$-norm of each prototype row is thus a measure of the certainty of the layer choice and increases as the search progresses. The condition for triggering the prototype inversion can then be a threshold on the $L_2$-norm of the prototype, averaged over all the rows (as they are assumed independent). If the inversion is used, this condition is checked at every iteration after the prototype is updated. The newly added uniformly distributed rows are ignored for the purposes of the mean norm calculation.

The inversion operation is implemented by subtracting each probability value from 1 (e.g. 0.85 becomes 0.15), followed by the same normalization as in probability capping, to ensure that each vector still sums to 1. We consider two types of inversion operation - the full inversion and the partial inversion. The former is applied row by row to the whole prototype. The latter is less destructive as it only applies to the subset of prototype rows which have the highest $L_2$-norm. The specific number of such rows is empirically set to $\lfloor \sqrt{N} \rfloor$. The partial inversion thus applies only to some of the most converged layers, preserving less confident choices as they are.

As both described techniques are simple mathematical operations on the prototype matrices, they do not incur significant computational costs by themselves. However, as they influence the search behaviour of the algorithm towards slowing down the convergence, more iterations may be required until the specific level of complexity is reached. With respect to this stopping condition, the proposed techniques can indirectly increase the overall running time of the algorithm, although the specific impact can only be evaluated empirically on a case-by-case basis.

IV. EXPERIMENTAL RESULTS AND ANALYSIS

In this section, we describe the experimental setting and obtained results and discuss their implications for this and future work.

A. Experimental Setting

Following the previous works, the proposed ASED algorithm is validated on the image classification problem. CIFAR-10 and CIFAR-100 datasets [64] have become a standard benchmark in the field. Both datasets feature 3-channel 32x32 RGB images, of which there are 50K training examples and 10K test examples. CIFAR-10 and CIFAR-100 contain 10 and 100 different classes, respectively. We choose to focus on CIFAR-100 as a more difficult multiclass problem. To allow for evaluation of candidate networks, we additionally split the original 50K training images into training and validation sets with 40K and 10K examples, respectively, preserving the class balance. This split is kept fixed throughout the experiments. The test set is used only to report the performance of the final discovered model. Classification accuracy is used as the performance metric. Standard CIFAR preprocessing is applied: images are padded by 4 pixels on each side, followed by random cropping down to 32x32 and horizontal flipping with probability 0.5, as well as normalization to zero mean and unit variance.

The algorithm parameters are set as follows. The search is initialized by sampling 10K networks from the uniform 5-layer prototype, which covers 10% of the design space (as the current library permits $10^5$ possible 5-layer networks). At every iteration of the search, $K = 1000$ networks are sampled, trained, and ranked, with the top $K_t = 100$ forming the next prototype. As adding layers is initially affordable, but becomes more expensive later, the following growth schedule is adopted:

$$n_t = \begin{cases} 2 & \text{if } t \in \{1, 2\} \\ 1 & \text{otherwise} \end{cases}$$ (4)

During the search, the channel count of all convolutional layers is set to 32. To avoid the mismatch of signal dimensions, every convolutional layer has its output padded to match the input; therefore, only the pooling layers can perform downsampling. We use PReLU as an activation function and apply the corresponding initialization policy of He et al. [65]. To make the discovered architectures output the class predictions, we perform global average pooling after the last sampled layer, followed by a fully connected layer of 100 PReLU-activated neurons, dropout with rate 0.5, and a softmax layer. We do not use batch normalization during the search; however, the final discovered architecture has batch normalization applied after every convolutional layer for evaluation purposes.

Training numerous deep networks from scratch incurs the majority of computational expenses of the search procedure. This leads us to utilize two different regimes – short training and long training. The former is used during all the steps of the search, including initialization and intermediate candidate
Fig. 1. Distributions of validation accuracies on CIFAR-100 (short training mode). The line plots show the maximum and median accuracies of the sampled networks.

ranking, while the latter is only applied to the evaluation of the final discovered architectures after the algorithm is run. Both settings use stochastic gradient descent (SGD) with momentum of 0.9 to minimize the cross entropy loss. Short training runs for 20 epochs, using the learning rate of $10^{-2}$ for the first 10 epochs and $10^{-3}$ thereafter. The long training runs for 200 epochs and uses the following schedule of learning rates: 0.01 for epochs 1-60, 0.02 for epochs 61-120, 0.004 for epochs 121-160, and 0.001 for epochs 161-200. Long training also uses $L_2$-norm weight regularization with the coefficient of $10^{-4}$ and imposes the maximum $L_2$-norm constraint of 0.5 on weights. The batch size is always set to 128.

All of our experiments are implemented in PyTorch and performed on a workstation with 4 GeForce 1080Ti GPU units. The running times are included with the reported results.

B. Architecture Search Performance

We report the results of running the proposed ASED algorithm on CIFAR-100 with the parameters described above. Four variants of the algorithm are tested: the baseline (Alg. 1), the variant with probability capping (denoted ProbCap for clarity), the full inversion variant, and the partial inversion variant. For ProbCap the maximum probability $p_{\text{max}}$ is set to 0.9. Both full inversion and partial inversion use the $L_2$-norm threshold of 0.65, as that corresponds to the middle of the interval of the possible values. The total number of iterations is $t_{\text{max}} = 9$ for the baseline and ProbCap variants, which, under the adopted schedule, corresponds to the maximum layer count of 16. However, for the inversion experiments the search is run further to allow for observation of the results after multiple instances of inversion triggering. The achievable layer count is thus 22 for these variants. The results, as internally computed by the ASED algorithm (and therefore based on the short training setting), are shown in Fig. 1.

While the constrained evaluation setting allows for reasonable computational expenses during the search time, these results are not indicative of the achievable performance. To confirm this, we conducted an extended validation of the best discovered networks by adding batch normalization layers and using the long training schedule (see Section IV-A). In this comparison, we also include the best architecture in the initialization sample (from the 5-layer uniform prototype), as well as the best 16-layer architecture from 1000 uniformly random samples. Every configuration is trained from scratch with the convolution channel counts of 32, 64, 128, and 256. The results are reported in Table I. The indicated layer count includes only operational layers (not identities). The discovered network structures are shown in Fig. 2.

The experiments confirm that the discovered architectures indeed perform better than their validation accuracy values would imply without context. Another observation is that the discovered networks do not reach the largest possible depth, despite the potential for further accuracy gains. If the evolution of the prototype reaches a point where the newly added layer assigns the largest probability to an identity operation, adding further layers is unlikely to introduce structural novelty, as they would also tend to converge to identities. The search essentially stops at that point. All of the algorithm variants demonstrate this behaviour, although the inversion variants are capable of avoiding it to a limited extent by setting the
Table I
Extended (long training + batch normalization) comparison of best discovered architectures by their test accuracy on CIFAR-100 dataset

| Model Source | Layer Count | 32 channels | 64 channels | 128 channels | 256 channels |
|--------------|-------------|-------------|-------------|--------------|--------------|
|              | Acc. | Par. | Acc. | Par. | Acc. | Par. | Acc. | Par. | Acc. | Par. |
| Initialization | 5 | 0.4898 | 221K | 0.5835 | 683K | 0.6419 | 2.4M | 0.6846 | 8.7M |
| Random uniform | 15 | 0.5794 | 443K | 0.6621 | 1.3M | 0.7200 | 4.4M | 0.7499 | 15.6M |
| ASED | 10 | 0.5659 | 319K | 0.6582 | 1.1M | 0.7102 | 3.9M | 0.7483 | 14.8M |
| ASED + Prob Cap | 8 | 0.5659 | 319K | 0.6582 | 1.1M | 0.7102 | 3.9M | 0.7483 | 14.8M |
| ASED + Full Inversion | 12 | 0.5827 | 504K | 0.6728 | 1.5M | 0.7297 | 5.1M | 0.7729 | 18.7M |
| ASED + Partial Inversion | 11 | 0.5748 | 471K | 0.6641 | 1.4M | 0.7249 | 4.6M | 0.7652 | 16.6M |

---

![Fig. 2. Best discovered structures for a) base procedure, b) probability capping, c) full inversion, d) partial inversion.](image)

identity probability low for previously discovered layers. The source of the issue lies in the evaluation procedure, as the results of Fig. [1] suggest that the range of validation accuracy is highly compressed. The short training schedule biases the search towards architectures that show the fastest improvement in early epochs. This can be advantageous if such a property is desirable, but it appears to make the architectures not competitive when a certain level of complexity is reached. On the other hand, as the explored networks grow in size, their training also becomes more demanding, making the short schedule a necessity for keeping the computational costs low. There exist multiple options to resolve this problem. Performance predictor can be trained to produce an approximate ranking of networks just from their structures, allocating training resources only to the most promising architectures (similar to [35]). Dynamic resource allocation scheme can be put in place to effectively manage the number of training epochs based on the network performance so far, assigning more computation to the models that demand it (see e.g. [66]). Finally, extension of the representation to support arbitrary connections can also alleviate the problem due to the less restricted flow of gradients [2]. We leave the research in this direction for the future work.

Among the tested variants the probability capping demonstrates inferior results, as the search process stagnates in the early stages. The superiority of the base search indicates that the convergence of individual probabilities to their extremes is actually desirable in the given formulation. Despite suboptimal local minima still being a concern, fixing some layers counter-balances the ever-growing dimensionality of the problem and allows for easier navigation of the design space. Inversion, on the other hand, improves the exploration capability of the search and empirically allows for the discovery of the superior architectures.

Table II presents the comparison between the ASED algorithm (the architecture discovered with the full inversion variant) and existing solutions with published results on CIFAR-100. The achieved accuracy is competitive, despite some limitations discussed above, as well as the fact that we neither utilize the reduced cell-based search space nor allow non-linear connectivity patterns, while offering an easier interpretability. The depth of networks produced by our method is currently limited, leaving room for further accuracy improvements. While the computational costs of our method are not among the lowest due to the large number of networks to train, it is worth noting that the evaluation step is easily parallelizable across any number of workers, due to each model being independent.
| Method              | Accuracy (%) | Parameter count | Model depth | Search cost (GPU days) |
|---------------------|--------------|-----------------|-------------|------------------------|
| FractalNet          | 76.7         | 38.6M           | 21          | N/A                    |
| Shake-Shake         | 84.2         | 26.2M           | 26          | N/A                    |
| Wide ResNet 28-10   | 80.4         | 36.5M           | 28          | N/A                    |
| DenseNet-BC         | 82.8         | 25.6M           | 190         | N/A                    |
| Genetic CNN         | 70.9         | –               | 17          | 17                     |
| MetaQNN             | 72.9         | 11.2M           | 9           | 100                    |
| Large Scale Evolution | 77.0     | 40.4M           | ≥ 13        | ≥ 2600                 |
| SMASH               | 79.4         | 16M             | 211         | 1.5                    |
| Hill Climbing       | 76.6         | 22.3M           | 30          | 1                      |
| NSGA-NET-128        | 79.3         | 3.3M            | 21          | 8                      |
| NSGA-NET-256        | 80.2         | 11.6M           | 21          | 8                      |
| ASEED               | 77.29        | 18.7M           | 12          | 20                     |

V. Conclusion

The automated neural architecture design is growing in importance as the application-driven demand outpaces the available expertise and resources. The probabilistic representation of the deep network structure that we propose has the advantages of being intuitive, easy to interpret and analyze, as well as readily extensible to incorporate many well-known elements of the field. While the optimization approach we consider is simple and limited in scale with respect to depth and computation, it is already capable of discovering competitive architectures, compared to existing methods with much higher methodological complexity and expressive search spaces.

The prototype-based approach is highly extensible and allows for many promising directions for future work. One possible direction is to increase the representation capability of the method to more closely match techniques from other works, such as supporting arbitrary inter-layer connections (possibly by using another, connectivity-specific prototype) and repeatable cells. Another direction could be the use of multiple prototypes simultaneously; while computational costs would need to be carefully managed, the ability to explore various regions of the design space simultaneously can lead to the discovery of unseen novel architectures and the higher robustness against premature convergence. Finally, the assumption of full layer independence can be dropped to explicitly model the structural patterns. For instance, the prototype could be comprised of joint probabilities of consecutive layers, yielding a bivariate distribution. As stated before, such flexibility is one of the major advantages of the proposed representation.

References

[1] Y. LeCun, Y. Bengio, and G. Hinton, “Deep learning,” Nature, vol. 521, no. 7553, pp. 436–444, 5 2015.
[2] K. He, X. Zhang, S. Ren, and J. Sun, “Deep Residual Learning for Image Recognition,” in Proceedings of the IEEE conference on Computer Vision and Pattern Recognition (CVPR), 2016, pp. 777–786.
[3] G. Huang, Z. Liu, L. Van Der Maaten, and K. Q. Weinberger, “Densely connected convolutional networks,” in IEEE Conference on Computer Vision and Pattern Recognition (CVPR), 2017, pp. 2261–2269.
Anton Muravev received his B.Sc. and M.Sc. degrees in computer science from the Tomsk Polytechnic University, Tomsk, Russia, followed by the M.Sc. degree in information technology from the Tampere University of Technology in 2013, 2015 and 2016 respectively. He is currently working towards the Ph.D. degree at the Tampere University, Tampere, Finland. His research interests include deep learning, pattern recognition and evolutionary computation.

Jenni Raitoharju is a postdoctoral research fellow at the Faculty of Information Technology and Communication Sciences, Tampere University, Finland. She received her PhD in Information Technology at Tampere University of Technology (TUT), Tampere, Finland in 2017. She has done research on different topics in machine learning and pattern recognition, such as stochastic optimization and different neural network models. Currently, she supervises research in several projects dealing with topics such as intelligent buildings, autonomous boats, and color constancy. She has 32 publications in peer-reviewed scientific journals (11) and conferences (21) (Google Scholar: 330+ citations, h-index 10). She was selected to Young Academy Finland (YAF) for 2018-2022 and to the board of YAF for 2018-2019. Recently, she received Academy of Finland Postdoctoral Researcher funding for 2019-2022.

Moncef Gabbouj received his MS and PhD degrees in electrical engineering from Purdue University, in 1986 and 1989, respectively. Dr. Gabbouj is a Professor of Signal Processing at the Department of Computing Sciences, Tampere University, Tampere, Finland. He was Academy of Finland Professor during 2011-2015. His research interests include Big Data analytics, multimedia content-based analysis, indexing and retrieval, artificial intelligence, machine learning, pattern recognition, nonlinear signal and image processing and analysis, voice conversion, and video processing and coding. Dr. Gabbouj is a Fellow of the IEEE and member of the Academia Europaea and the Finnish Academy of Science and Letters. He served as associate editor and guest editor of many IEEE, and international journals.