ABSTRACT
The computational demands of neural architecture search (NAS) algorithms are usually directly proportional to the size of their target search spaces. Thus, limiting the search to high-quality subsets can greatly reduce the computational load of NAS algorithms. In this paper, we present Clustering-Based REDuction (C-BRED), a new technique to reduce the size of NAS search spaces. C-BRED reduces a NAS space by clustering the computational graphs associated with its architectures and selecting the most promising cluster using proxy statistics correlated with network accuracy. When considering the NAS-Bench-201 (NB201) data set and the CIFAR-100 task, C-BRED selects a subset with 70% average accuracy instead of the whole space’s 64% average accuracy.

CCS CONCEPTS
• Computing methodologies → Machine learning approaches.

KEYWORDS
deep learning, neural architecture search, training-free statistics, computational graph, clustering

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1 INTRODUCTION
Deep neural networks (DNNs) have been breaking accuracy records in diverse fields, from computer vision to natural language processing. However, designing new task-accurate architectures requires considerable expertise, time, and computing resources. NAS aims at accelerating the development of accurate DNNs by parametrising network designs and automating the selection of optimal networks. The basic working principle of NAS is simple: given a collection of candidate network architectures (the NAS space), apply a procedure that can select the best performing one (the NAS algorithm) [3].

Most NAS approaches have huge computational requirements [9, 11]. Empirical evidence suggests that both the convergence time and the final performance of NAS algorithms depend on the size of the search space and the accuracy distribution of its enclosed networks, with smaller and high-performing spaces having the advantage [2, 4, 8]. Thus, the deep learning community has devoted significant efforts to understanding search spaces and designing increasingly better ones. However, the proposed techniques either lack full automation or require training large amounts of networks [2, 8]. Some NAS algorithms include search space selection in their optimisation loop, but this selection is either not independent of the search algorithm [4] or uses extremely simple heuristics [6].

In this work, we provide the following contributions to NAS.

• We present C-BRED, an unsupervised technique to restrict NAS spaces to high-performing subsets. C-BRED combines pointwise information (proxy statistics) with relational information (clustering of computational graphs) about network architectures to identify high-quality subsets of the target NAS space without requiring any training iteration.
• We demonstrate C-BRED’s effectiveness on the NB201 space, where it identifies a subset with 70% average CIFAR-100 accuracy, as opposed to the baseline 64% of the whole space.

2 BACKGROUND AND FORMULATION
We model the architectures from a given NAS space using a latent variable $\lambda \in \Lambda$. Each architecture manifests itself in two forms: the function form $f_\lambda$ and the program form $G_\lambda$.

2.1 Training-free statistics
In its function form, each architecture is a parametric function $f_\lambda : \Theta_\lambda \times X \rightarrow Y$, where $X$ is the input space, $Y$ is the output space, and $\Theta_\lambda$ is the parameter space. Given an initial condition $\theta_0^{(T)}$, training a network amounts to defining a path $(\theta_0^{(0)}, \ldots, \theta_0^{(T)})$ in the parameter space. In each state of such a path, statistics about $f_\lambda$ can be measured. The most important statistic is task accuracy, which is measured at the end of training ($\theta_\lambda = \theta_0^{(T)}$). Recent NAS
research has identified training-free (TF) statistics, i.e., statistics that can be measured ahead of training ($\theta_j = \theta_j^{(0)}$) and correlate with the network’s task accuracy. Examples of TF statistics are the condition number of the neural tangent kernel, the number of linear regions cut by a ReLU-activated network in its input space, and the so-called NAS-without-training (NASWOT) statistics [1, 7].

2.2 Computational graphs
In its program form, each architecture is a computational graph $G_\lambda = (M_\lambda \cup K_\lambda, R_\lambda \cup W_\lambda)$, where $M_\lambda$ is a set of memory nodes, $K_\lambda$ is a set of kernel nodes, $R_\lambda \subset M_\lambda \times K_\lambda$ contains read operations, and $W_\lambda \subset K_\lambda \times M_\lambda$ contains write operations. This interpretation exposes how the information flows through DNNs and allows to characterise the workload that they impose on the underlying computing platform [5]. Note that DNN computational graphs can be encoded in different ways, as surveyed in [10].

3 CLUSTERING-BASED REDUCTION
Given a NAS space $\Lambda$, our objective is to identify $\Lambda' \subset \Lambda$ such that $|\Lambda'| \ll |\Lambda|$ and the average quality of networks in $\Lambda'$ is better than that of the networks in $\Lambda$. C-BRED achieves this goal as follows:

(1) define a similarity measure $d(G_{\lambda_1}, G_{\lambda_2}) \geq 0$ over the program forms $G_{\lambda}$;
(2) cluster $\Lambda$ into a collection $\{\Lambda_1, \ldots, \Lambda_{K}\}$ ($K \geq 2$) of candidate subsets using the similarity measure;
(3) measure TF statistics for all the program forms $f_\lambda$ in each candidate subset;
(4) select $\Lambda^* = \Lambda_{k^*}$ by means of a selector function combining the values of the TF statistics of the architectures inside each candidate cluster and comparing the aggregated results.

C-BRED is actually a meta-algorithm in that the graph similarity measure and the cluster selector function can be tuned.

4 EXPERIMENTAL RESULTS
We evaluated C-BRED on the NB201 benchmark search space.
NB201 contains 5380 unique cell-based architectures: each architecture is built by generating a smaller network (the cell), replicating it several times, and composing the replicas. This property allows simplifying computational graph comparisons since we can compare two architectures by comparing their originating cells. To compare two cells, we defined two similarity measures: the first one is topology-agnostic and compares the frequency with which each kernel type (e.g., convolution, skip connection) is used in the cell; the second one compares instead how many times a given kernel type is used as part of a computational path. We clustered program forms using the DBSCAN algorithm and empirically found that a combination of the two distances works best. Our selector function is a heuristic combining all the four TF statistics proposed in [1] and [7] (both versions). We developed such a function by analysing a data set of TF statistics that we created for NB201.

The average CIFAR-100 accuracy of NB201 networks is 64%, whereas that of the networks in the subset selected by C-BRED is 70%. To validate this preliminary evaluation, we compared C-BRED to two subspace selection alternatives. The alternatives we chose partition NB201 into five subsets according to the 20% quantiles associated with two statistics: the NASWOTv2 statistic and the number of multiply-accumulate (MAC) operations. We then used the NASWOT technique introduced in [7] as the reference search algorithm. As can be seen in Table 1, C-BRED has superior performance in that not only the average network accuracy is better, but it is also more stable ($\sim 4\times$ decrease in standard deviation).

|                      | Intrinsic | TF-Q  | MAC-Q  | C-BRED |
|----------------------|-----------|-------|--------|--------|
| Mean                 | 69.18     | 69.54 | 69.86  | 70.34  |
| Median               | 69.60     | 69.90 | 70.16  | 70.23  |
| Standard deviation   | 1.93      | 1.74  | 1.47   | 0.41   |

5 CONCLUSIONS
In this paper, we presented C-BRED, a technique to identify subsets of NAS spaces containing high-quality architectures. C-BRED uses relational information about computational graphs to cluster the target NAS space into a collection of candidate subsets; then, it uses pointwise information (TF statistics) to identify the most promising cluster without requiring any training iteration.

REFERENCES
[1] Wuyang Chen, Xinyu Gong, and Zhangyang Wang. 2021. Neural architecture search on ImageNet in four GPU hours: a theoretically inspired perspective. In Proceedings of the 9th International Conference on Learning Representations (ICLR 2021). ICLR.
[2] Yuanzheng Ci, Chen Lin, Ming Sun, Boyu Chen, Hongwen Zhang, and Wanli Ouyang. 2021. Evolving search space for neural architecture search. In Proceedings of the 2021 IEEE/CVF International Conference on Computer Vision (ICCV 2021). IEEE.
[3] Thomas Elsken, Jan H. Metzen, and Frank Hutter. 2019. Neural architecture search: a survey. Journal of Machine Learning Research 20 (2019), 1–21.
[4] Yiming Hu, Yudong Liang, Zachao Guo, Ruosi Wan, Xiangyu Zhang, Yichen Wei, Qiangyi Gu, and Jan Sun. 2020. Angle-based search space shrinking for neural architecture search. In Proceedings of the 16th European Conference on Computer Vision (ECCV 2020). ACM.
[5] Edgar Liberis, Lukasz Dudziak, and Nicholas D. Lane. 2021. $\mu$NAS: constrained neural architecture search for microcontrollers. In Proceedings of the 1st Workshop on Machine Learning and Systems (EuroMLSys ’21). ACM.
[6] Ji Lin, Wei-Ming Chen, Yujun Lin, John Cohn, Chuang Gan, and Song Han. 2020. MCUNet: tiny deep learning on IoT devices. In Proceedings of the 34th Conference on Neural Information Processing Systems (NeurIPS 2020). Neural Information Processing Systems.
[7] Joseph Mellor, Jack Turner, Amos Storkey, and Elliott J. Crowley. 2021. Neural architecture search without training. In Proceedings of the 38th International Conference on Machine Learning (ICML 2021). MLResearchPress.
[8] Ilja Radasavovic, Raj P. Kosaraju, Ross Girshick, Kaiming He, and Piotr Dollar. 2020. Designing network design spaces. In Proceedings of the 2020 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR 2020). IEEE.
[9] Mingxing Tan, Bo Chen, Ruoming Pang, Vijay Van Belleghem, Mark Sandler, Andrew Howard, and Quoc V. Le. 2019. MnasNet: platform-aware neural architecture search for mobile. In Proceedings of the 2019 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR 2019). IEEE.
[10] Colin White, Willie Neiswanger, Sam Nolen, and Yash Sabani. 2020. An study on encodings for neural architecture search. In Proceedings of the 34th Conference on Neural Information Processing Systems (NeurIPS 2020). Neural Information Processing Systems.
[11] Bichen Wu, Xiaolong Dai, Peizhao Zhang, Yanghang Wang, Fei Sun, Yiming Wu, Yuandong Tian, Peter Vajda, Yangqing Jia, and Kurt Keutzer. 2018. FIBNet: hardware-aware efficient ConvNet design via differentiable neural architecture search. In Proceedings of the 2018 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR 2018). IEEE.