Dextr: Zero-Shot Neural Architecture Search with Singular Value Decomposition and Extrinsic Curvature

Anonymous authors
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Abstract

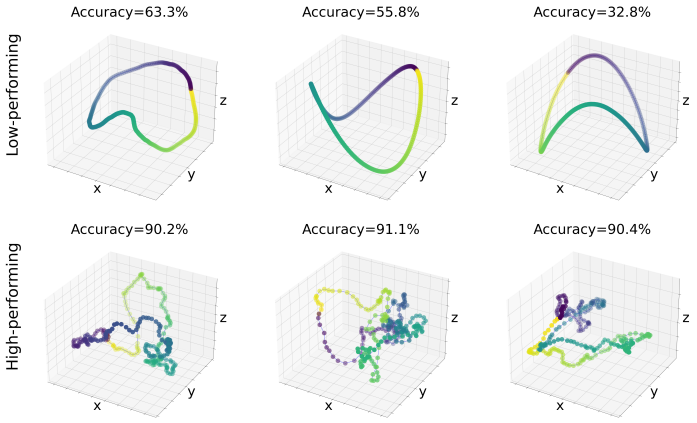
Zero-shot Neural Architecture Search (NAS) typically optimises the architecture search process by exploiting the network or gradient properties at initialisation through zero-cost proxies. The existing proxies often rely on labelled data, which is usually unavailable in real-world settings. Furthermore, the majority of the current methods focus either on optimising the convergence and generalisation attributes or solely on the expressivity of the network architectures. To address both limitations, we first demonstrate how channel collinearity affects the convergence and generalisation properties of a neural network. Then, by incorporating the convergence, generalisation and expressivity in one approach, we propose a zero-cost proxy that omits the requirement of labelled data for its computation. In particular, we leverage the Singular Value Decomposition (SVD) of the neural network layer features and the extrinsic curvature of the network output to design our proxy. Our approach enables accurate prediction of network performance on test data using only a single label-free data sample. Our extensive evaluation includes a total of six experiments, including the Convolutional Neural Network (CNN) search space, i.e. DARTS and the Transformer search space, i.e. AutoFormer. The proposed proxy demonstrates a superior performance on multiple correlation benchmarks, including NAS-Bench-101, NAS-Bench-201, and TransNAS-Bench-101-micro; as well as on the NAS task within the DARTS and the AutoFormer search space, all while being notably efficient.

1 Introduction

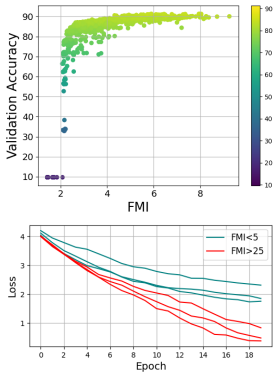
Following the success of standard deep neural network architectures (He et al., 2016; Szegedy et al., 2015; LeCun et al., 1998; Vaswani et al., 2017), the search for optimal network topologies, referred to as Neural Architecture Search (NAS), has gained significant attention in the past years. Search-based (Li & Talwalkar, 2020; White et al., 2021), reinforcement learning methods (Zoph & Le, 2017; Tian et al., 2020), as well as evolutionary algorithms (Real et al., 2019; Chu et al., 2020a) have originally been used to tackle this task. However, they suffer from heavy computational requirements due to the enormous search space. Generative methods (Lukasik et al., 2022; Asthana et al., 2024; An et al., 2024) alleviate this issue by deploying gradient-based learning of the search space through first-order methods. However, the requirement for architectural training data, including the performance of each architecture, poses a serious challenge to the applicability of these methods in practice. Alternatively, zero-shot NAS eliminates the need for such an architecture dataset. This technique leverages the network structure and gradient properties close to initialisation (termed as zero-cost proxies) to predict the performance on a test set prior to its full training (Abdelfattah et al., 2021).

Normally, zero-cost proxies are either task/data agnostic, e.g. FLOPS or parameters, or data-based. While most of the data agnostic proxies (Tanaka et al., 2020; Lin et al., 2021; Li et al., 2021b) fail to be consistent, most data-dependent proxies (Mellor et al., 2021; Abdelfattah et al., 2021) require labels for gradient computation, which are usually not available in real-world scenarios. Thus, these drawbacks motivate the design of a zero-cost proxy independent of labelled data.

Another limitation of most current proxies is their focus on performance attributes that they aim to optimise. Formally, network performance is analysed through three attributes, namely convergence, generalisation,



(a) Outputs of six randomly initialised networks induced by a circular input projected on the first three principal components. The accuracies are reported with respect to training on CIFAR-10.



(b) (top) Scatter plot between the network performance and linear independence of feature maps (FMI). (bottom) Training loss curve for six networks sampled from NAS-Bench-201 on CIFAR-10.

Figure 1: Comparison of convergence, generalisation, and expressivity of low-performing and high-performing networks sampled from NAS-Bench-201 (Dong & Yang, 2020). (a) **Expressivity:** The outputs of the high-performing networks projected on the first three principal components induced by an arbitrary circular input are more curved than those of the low-performing networks. Hence, the low-performing networks are less expressive than the high-performing networks. (b-top): **Generalisation:** The linear independence of feature maps (FMI) is positively correlated to the validation accuracy and hence, generalisation of the network. (b-bottom): **Convergence:** The networks with high FMI (FMI>25) demonstrate faster convergence during training on CIFAR-10.

and expressivity (Chen et al., 2023). Convergence refers to how fast a network can converge to a minimum through gradient descent. Generalisation refers to how well a network trained on training data can generalise to unseen test data. Finally, expressivity indicates the complexity of functions that a network can estimate. In addition, the No Free Lunch theorem states that the most optimal network balances these attributes as it is practically impossible to minimise all three simultaneously (Chen et al., 2023). Most zero-cost proxies focus either on convergence and generalisation aspects (Jiang et al., 2023; Li et al., 2023; Yang et al., 2023) or solely on the expressivity characteristic (Lin et al., 2021). However, designing a proxy by balancing all three attributes is an open challenge that is hardly addressed in the literature (Lee & Ham, 2024).

To address the above shortcomings, we present a zero-cost proxy that (i) operates without the need for labelled data, and (ii) balances convergence, generalisation, and expressivity of networks in one approach. To this end, we first demonstrate using Singular Value Decomposition (SVD) (Klema & Laub, 1980) that the collinearity of feature maps negatively affects the training convergence rate and generalisation capabilities of a Convolutional Neural Network (CNN). In other words, the convergence and generalisation of a CNN are positively correlated to the linear independence of feature maps (FMI), as illustrated in Figure 1b. Moreover, we employ Riemannian geometry (Lee, 2006) to consider the relationship between the extrinsic curvature of the output and the expressivity of a network (Poole et al., 2016). Specifically, we utilize the fact that the expressivity of a network is related to how curved the output is when an input is fed into the network. This is visually illustrated in Figure 1a. Based on the relationships related to convergence, generalisation, and expressivity, we propose a cost-effective proxy, namely Dextr, which leverages the collinearity of layer feature maps and the extrinsic curvature of the output. As a result, Dextr accurately predicts the network performance on test data using just a single label-free data sample. Our evaluation shows the capabilities of our proxy by outperforming all existing zero-shot NAS methods on three standard tabular benchmarks, specifically NAS-Bench-101 (Ying et al., 2019), NAS-Bench-201 (Dong & Yang, 2020), and TransNAS-Bench-micro (Duan et al., 2021) benchmarks, and showing competitive performance in the NAS-Bench-301 (Zela et al., 2022) benchmark. Additionally, we perform experiments within two search spaces: the DARTS

search space (Liu et al., 2019) containing CNNs, and the AutoFormer search space (Chen et al., 2021b) containing Vision Transformers (ViTs) (Dosovitskiy et al., 2021). The architecture discovered through our proxy in these search spaces is then evaluated by training it on ImageNet (Deng et al., 2009) and its test performance is compared with baseline approaches. We demonstrate that the architecture found through our proxy outperforms the previous multi-shot and zero-shot NAS methods on ImageNet classification, all while maintaining minimal search time. We conduct a total of three ablation studies, where we analyse the stability of our approach, compare Dextr with a simple combination of existing proxies, and analyse contribution of individual layers. We additionally perform two experiments on NATS-Bench-SSS (Dong et al., 2021) and MobileNet-v2 (Sandler et al., 2018), provided in the Appendix Section A.2. In summary, our contributions are as follows:

- We present the relationship between the collinearity of feature maps across a convolutional layer in a network and the convergence and generalisation capabilities of the network.
- By incorporating the convergence, generalisation, and expressivity in our proxy, we propose a zero-cost proxy requiring one label-free data sample for its computation.
- Our proposed proxy outperforms the existing methods on three correlation benchmarks, i.e. NAS-Bench-101 (Ying et al., 2019), NAS-Bench-201 (Dong & Yang, 2020), and TransNAS-Bench-101-micro (Duan et al., 2021), as well as on the ImageNet (Deng et al., 2009) NAS task within the DARTS (Liu et al., 2019) search space and the AutoFormer search space (Chen et al., 2021b).

2 Related Work

Multi-shot and Zero-Shot NAS Traditional attempts to automate the design process of neural network architectures, such as random search (Li & Talwalkar, 2020), evolutionary approaches (Real et al., 2019; Chu et al., 2020a), reinforcement learning approaches (Zoph & Le, 2017; Tian et al., 2020), and gradient-based approaches (Brock et al., 2018; Yang et al., 2020a; Chen et al., 2021d), are considered rather slow due to the requirement of training iterations at each search step (Liu et al., 2019). More recent generative methods (Lukasik et al., 2022; Asthana et al., 2024; An et al., 2024) addressed this limitation by employing learning-based techniques in the architecture search space. For instance, Lukasik et al. (2022) employed a generator and surrogate predictor to accurately learn and sample from the architectural data distribution. Recently, similar to this direction, An et al. (2024) and Asthana et al. (2024) employed conditioned diffusion models to generate well-performing neural network architectures. However, the expensive training process of the generative models and the requirement of architectural training data limits the applicability of these approaches.

Alternatively, zero-shot NAS accelerates the rather costly architecture search process (Li & Talwalkar, 2020; White et al., 2021; Zoph & Le, 2017; Tian et al., 2020; Real et al., 2019; Chu et al., 2020a) by using network metrics at initialisation, known as zero-cost proxies. The concept of zero-shot NAS was established by Mellor et al. (2021), who introduced the activation overlap between data points as a proxy. Since then, various zero-cost proxies (Lee et al., 2019; Lin et al., 2021; Chen et al., 2021c) have advanced the field, including Snip (Lee et al., 2019), Grasp (Wang et al., 2020), Synflow (Tanaka et al., 2020), Fisher (Turner et al., 2020), and Jacob (Mellor et al., 2021), all proposed by Abdelfattah et al. (2021). Additionally, Li et al. (2023) have introduced ZiCo , which predicts network performance using the mean and standard deviation of parameter gradients at initialisation. Unlike our approach, all these proxies rely on data labels for their computation.

In contrast, some previous works do not require data labels for performance estimation. For instance, NASWOT (Mellor et al., 2021) analyses activation overlaps for network performance estimation. However, it only considers the expressivity of a network and neglects the convergence and generalisation attributes. Similarly, Zen (Lin et al., 2021) considers the expressivity exclusively by utilising the network's Gaussian complexity. Conversely, MeCo (Jiang et al., 2023) omits the need for labels by calculating the minimum eigenvalue of the Pearson Correlation matrix. However, it solely focuses on the convergence and generalisation aspects of the network, while neglecting the expressivity. To consider all three attributes, Chen et al. (2021c) utilised Neural Tangent Kernels (NTK) and the Number of Linear Regions (NLR) for efficient architecture

search. More recently, AZ-NAS (Lee & Ham, 2024) considers multiple network attributes like trainability, expressivity, progressivity, and complexity. However, they both require labels and backpropagation for their calculation. Following a more efficient direction, we propose a zero-cost proxy that further improves the performance without requiring labels while considering all three performance attributes, i.e. convergence, generalisation, and expressivity.

Performance Attributes Several works have studied the theory concerning convergence, generalisation and expressivity of the neural networks (Neal, 1996; Williams, 1996; Du et al., 2019a; Poole et al., 2016). For instance, Du et al. (2019a;b) provided insights into the convergence and generalisation of overparameterized networks through gram matrix analysis. Building upon this idea, we establish a connection between the collinearity of feature maps and the convergence and generalisation capabilities of CNNs. Additionally, Poole et al. (2016) investigated the expressivity of neural networks using concepts from Riemannian geometry (Lee, 2006) and Mean Field Theory (Weiss, Pierre, 1907). We leverage these concepts to incorporate expressivity into our proxy. Finally, Chen et al. (2023) demonstrated the 'No Free Lunch' behaviour, indicating that with a fixed number of parameters, no single architecture can simultaneously optimise all performance attributes. This is because convergence and generalisation properties favour wide and shallow networks while expressivity favours deep and narrow network topologies. Hence, our proxy aims to balance these attributes rather than optimising all three simultaneously.

3 Dextr

3.1 Problem Formulation

Consider the convergence, generalisation, and expressivity of an overparameterised neural network. In this context, convergence refers to the rate at which the loss of this network reaches a minimum, generalisation refers to the performance of the network on unseen test data post-training, and expressivity refers to the ability of the network to model complex functions.

We aim to design a zero-cost proxy that considers all three attributes – convergence, generalisation, and expressivity of a network without the requirement for labelled data. To this end, based on the background concepts detailed in Section 3.2, we establish the relationship between the collinearity of feature maps of a specific convolutional layer in the CNN with the convergence and generalisation properties of this network, by employing Singular Value Decomposition. To address expressivity, we build upon the findings of Poole et al. (2016) (Section 3.2.2) for designing our proxy. Next, we apply our proposed proxy to Vision Transformers (ViTs) (Section 3.3.4). Finally, we utilise the proposed proxy to search for optimal neural architectures in a training-free setting.

3.2 Background Theory

We consider, for simplicity, the two-layer fully-connected neural network $f(\mathbf{W}, \mathbf{a}, \mathbf{x}_i)$ with ReLU activation function, as Du et al. (2019b), such that

$$f(\mathbf{W}, \mathbf{a}, \mathbf{x}_i) = \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r \sigma(\mathbf{w}_r^T \mathbf{x}_i), \tag{1}$$

where $\mathbf{x}_i$ is the input to f taken from the training set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, y_i is the ground-truth for $\mathbf{x}_i$, $\mathbf{w} \in \mathbb{R}^d$ and $\mathbf{W} \in \mathbb{R}^{d \times m}$ are the weight vector and matrix for the first layer respectively, m is the number of hidden nodes, σ is the ReLU activation function, $a_r \in \mathbb{R}$ is the output weight, and $\mathbf{a} \in \mathbb{R}^{m \times 1}$ is the output weight vector. We consider the simple case where the training objective of this network is to minimise the following Mean Squared Error (MSE) loss (Du et al., 2019b):

$$L(\mathbf{W}, \mathbf{a}) = \sum_{i=1}^{n} \frac{1}{2} (f(\mathbf{W}, \mathbf{a}, \mathbf{x}_i) - y_i)^2. \tag{2}$$

First, we present the background theory regarding convergence, generalisation, and expressivity of f. Then, we demonstrate the transferability of these foundational concepts to CNNs.

3.2.1 Convergence and generalisation: Minimum eigenvalue of gram matrix

We start by examining the convergence and generalisation of f. Following Du et al. (2019b), consider a continuous training scenario where f is trained through gradient descent with infinitely small step-size t, and the output layer of f is fixed. The prediction of this network on a given input $\mathbf{x}_i$ at training time step t is denoted as $u_i(t) = f(\mathbf{W}(t), \mathbf{a}, \mathbf{x}_i)$. Then, the gram matrices generated by the ReLU activation function on the training set $\mathcal{D}$ at a given time t and at initialisation, i.e. $t = 0$, respectively are defined as

$$[\mathbf{H}(t)]_{ij} = \frac{1}{m} \sum_{r=1}^{m} \mathbf{x}_i^T \mathbf{x}_j \mathbb{I}\{\mathbf{w}_r^T(t)\mathbf{x}_i \geq 0, \mathbf{w}_r^T(t)\mathbf{x}_j \geq 0\},$$

$$\mathbf{H}_{ij}^{\infty} = \mathbb{E}_{\mathbf{w}\sim\mathcal{N}(\mathbf{0},\mathbf{I})}[\mathbf{x}_i^T \mathbf{x}_j \mathbb{I}\{\mathbf{w}^T\mathbf{x}_i \geq 0, \mathbf{w}^T\mathbf{x}_j \geq 0\}],$$

where $r \in [m]$, $\mathcal{N}\{\cdot\}$ represents the Gaussian distribution, $\mathbb{I}$ represents the indicator function and $\mathbf{H}(t) \in \mathbb{R}^{n\times n}, \mathbf{H}^{\infty} \in \mathbb{R}^{n\times n}$ are the respective gram matrices. Next, we consider the following theorem for network convergence (Du et al., 2019b).

Theorem 1 *Let the input be $i \in [n]$, $c_{low} < \|\mathbf{x}_i\|_2 < c_{high}$ and $\|y_i\| < C$, where c_{high}, c_{low}, and C are constants. If the number of nodes m is set to $\Omega(\frac{n^6}{\lambda_{min}(\mathbf{H}^{\infty})^4\delta^6})$, where δ is the probability of failure, Ω denotes the lower bound, and $\lambda_{min}(\mathbf{H}^{\infty})$ denotes the scaled minimum eigenvalue of $\mathbf{H}^{\infty}$, and we i.i.d. initialise $\mathbf{w}_r \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and $a_r \sim \mathcal{U}\{[-1, 1]\}$, where $\mathcal{U}\{\cdot\}$ represents the uniform distribution, then with at least $1 - \delta$ probability, the following relationship holds:*

$$\|\mathbf{u}_i(t) - \mathbf{y}_i\|_2^2 \leq \exp(-\lambda_{min}(\mathbf{H}^{\infty})t)\|\mathbf{u}_i(0) - \mathbf{y}_i\|_2^2. \tag{3}$$

Theorem 1 establishes that the loss incurred by f at time-step t, defined as $\|\mathbf{u}(t) - \mathbf{y}\|_2^2$, has an upper bound controlled by $\lambda_{min}(\mathbf{H}^{\infty})$. This quantity measures the convergence rate of f when m is large. Thus, $\lambda_{min}(\mathbf{H}^{\infty})$ positively correlates with the convergence rate of f. The proof of this theorem is provided in the work by Du et al. (2019b). Next, we explore network generalisation based on the following theorem from Cao & Gu (2019) and Zhu et al. (2022).

Theorem 2 *Let the loss function of f with $m \to \infty$ evaluated on the test set be denoted as $L(\mathbf{W})$. Let the ground truth $\mathbf{y} = (y_1, ..., y_N)^T$, where N is the total number of samples and γ represents the step size of stochastic gradient descent (SGD), determined by $\gamma = kC_1\sqrt{\mathbf{y}^T(\mathbf{H}^{\infty})^{-1}\mathbf{y}}/(m\sqrt{N})$, where k is a sufficiently small absolute constant (Zhu et al., 2022). If Theorem 1 holds, then for any $\delta \in (0, e^{-1}]$, there exists a value m^* which depends on δ, N, and $\lambda_{min}(\mathbf{H}^{\infty})$ such that if $m \geq m^*$, with a probability of at least $1 - \delta$, the following inequality holds:*

$$\mathbb{E}[L(\mathbf{W})] \leq \mathcal{O}\left(C_2\sqrt{\frac{\mathbf{y}^T\mathbf{y}}{\lambda_{min}(\mathbf{H}^{\infty})N}}\right) + \mathcal{O}\left(\sqrt{\frac{\log(1/\delta)}{N}}\right), \tag{4}$$

where C_1 and C_2 are constants.

We notice from Theorem 2 that $\lambda_{min}(\mathbf{H}^{\infty})$ exhibits a negative correlation with the upper bound of the test loss, thereby indicating a positive correlation with the generalisation capabilities of f. The proof of this theorem is detailed in the work by Jiang et al. (2023).

Remark 1 *Based on Theorems 1 and 2 and findings from Du et al. (2019b), while $\mathbf{H}(t)$ changes through the progression of t from 0 to ∞, it still stays close if $m \to \infty$. Moreover, for any two non-parallel inputs $\mathbf{x}_i$ and $\mathbf{x}_j$ (i.e. $\mathbf{x}_i \nparallel \mathbf{x}_j$), the minimum eigenvalue of the gram matrix $\mathbf{H}^{\infty}$ at initialisation, i.e. $\lambda_{min}(\mathbf{H}^{\infty})$ is strictly positive, i.e. $\lambda_{min}(\mathbf{H}^{\infty}) > 0$, and is positively correlated to the convergence rate and generalisation capabilities of f.*

The relationship between $\mathbf{H}(t)$ and $\mathbf{H}^{\infty}$ in Remark 1 also implies that the inputs $\mathbf{x}_i(t)$ and $\mathbf{x}_j(t)$ at any training time step t can be used to estimate the convergence rate and generalisation of f. This motivates us to design our proxy close to the start of the training, i.e. when t is close to 0.

3.2.2 Expressivity: Extrinsic curvature of the output

Next, we consider the expressivity characteristics of f using the characterisation through extrinsic curvature of the output, given by Poole et al. (2016). To examine the expressivity of f, we leverage principles from Riemannian geometry (Lee, 2006). In this geometry, a manifold represents a topological space that resembles Euclidean space locally near each point but may have an intricate global structure. Following Poole et al. (2016), we define $\mathbf{g}(\theta)$ as a 1-dimensional manifold within the input space, where θ serves as an intrinsic scalar coordinate on this manifold. We consider $\mathbf{g}(\theta)$ to be an arbitrary circular input i.e. $\mathbf{g}(\theta) = \sqrt{N_1 q}[\mathbf{o}^0 cos(\theta) + \mathbf{o}^1 sin(\theta)]$, where $\theta \in [0, 2\pi)$, and $\mathbf{o}^0$, $\mathbf{o}^1$ form an orthonormal basis for a 2-dimensional subspace of $\mathbb{R}^{N_1}$. The layer propagation of f transforms this input manifold into a new manifold $\mathbf{h}^l(\theta) = \mathbf{h}^l(\mathbf{g}(\theta))$, where l corresponds to the layers of f. Each point θ in the manifold $\mathbf{h}^l(\theta)$ induces a velocity vector (equal to its tangent), represented by $\mathbf{v}^l(\theta) = \partial_\theta \mathbf{h}^l(\theta)$, and an acceleration vector $\mathbf{a}^l(\theta) = \partial_\theta \mathbf{v}^l(\theta)$. Formally, the extrinsic curvature of the output, induced by the arbitrary circular input $\mathbf{g}(\theta)$ parameterised by θ is defined as in Poole et al. (2016):

$$\kappa(\theta) = (\mathbf{v} \cdot \mathbf{v})^{-3/2} \sqrt{(\mathbf{v} \cdot \mathbf{v})(\mathbf{a} \cdot \mathbf{a}) - (\mathbf{v} \cdot \mathbf{a})^2}. \tag{5}$$

Remark 2 *The extrinsic curvature of the output, i.e. $\kappa(\theta) \in \mathbb{R}$ measures the complexity of the output curve, which indicates the functional complexity of f. Thus, $\kappa(\theta)$ is positively correlated to the expressivity characteristic of the network f.*

Intuitively, a more expressive network induces a more tangled output manifold after propagation through the network, as observed in Figure 1a. Thus it has a higher $\kappa(\theta)$. The extrinsic curvature $\kappa(\theta)$ remains invariant irrespective of the particular parameterisation θ and does not require any data for its computation. Moreover, this characterisation of expressivity is applicable to networks with random weights (Poole et al., 2016), i.e. at time-step $t = 0$. The data-independent property of $\kappa(\theta)$, as well as its ability to express the functional complexity of f at network initialisation makes it suitable to incorporate $\kappa(\theta)$ in our proxy.

3.2.3 Approximation to convolutional layer

Consider the multi-channel convolutional layer l^{cnn} of the CNN f_{cnn}. The number of channels in layer l^{cnn} is denoted as C. The vector-represented output feature maps at time step t are denoted as $\mathbf{x}_c^\phi(t)$, where $c \in \{1, 2, \cdots, C\}$. We define $\mathbf{X}^\phi(t)$ as a matrix containing all the vector-represented feature maps, such that $\mathbf{x}_c^\phi(t) \in \mathbf{X}^\phi(t)$. The network f_{cnn} is trained on the training set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$. The output of f_{cnn} at time step t is denoted as $\mathbf{u}_i^\phi(t)$ and the loss incurred by f_{cnn} at time step t is defined as $\|\mathbf{u}_i^\phi(t) - \mathbf{y}_i\|_2^2$.

Remark 3 *Through the approximation of the multi-sample fully-connected layer of f to a multi-channel convolutional layer l^{cnn} of the network f_{cnn} under some constraints presented by Jiang et al. (2023), we know that each data sample $\mathbf{x}_i$ can be regarded as a vector-represented channel $\mathbf{x}_c^\phi$ of the convolutional layer l^{cnn}, where $c \in \{1, C\}$. Thus, the concepts regarding f presented in Section 3.2.1 and 3.2.2 hold for f_{cnn} by replacing the input data sample $\mathbf{x}_i$ with the feature maps $\mathbf{x}_c^\phi$.*

Hence, the gram matrix $\mathbf{H}(t)$ for multiple input samples in the fully-connected layer of f can be approximated as $\mathbf{H}^\phi(t)$ for multiple channels in the convolutional layer l^{cnn}, where $\mathbf{H}^\phi(t)$ is the gram matrix associated to the feature maps at time step t.

3.3 Designing Dextr

We now design our zero-cost proxy, focused on CNNs (Sec. 3.2.3), by utilising the remarks on the convergence and generalisation (Sec. 3.2.1), as well as expressivity (Sec. 3.2.2). In particular, we exploit the collinearity (Sec. 3.3.1) among all channels of the layers in the CNN using SVD (Sec. 3.3.2) to formulate our proxy, namely Dextr.

3.3.1 Multi-collinearity in feature maps

According to Remark 1, we observe that firstly $\lambda_{min}(\mathbf{H}^{\infty})$ correlates positively with the training convergence rate and the generalisation capabilities of f. Furthermore, for any two non-parallel inputs $\mathbf{x}_i$ and $\mathbf{x}_j$, $\mathbf{H}(t)$ remains close to $\mathbf{H}^{\infty}$ at each training time step t. Therefore, when t is close to 0, $\lambda_{min}(\mathbf{H}(t))$ can similarly measure the convergence and generalisation of f. In Remark 3, we recall the approximation of a fully-connected layer to the convolutional layer (Jiang et al., 2023) by replacing the input sample $\mathbf{x}_i(t)$ with the vector-represented channel $\mathbf{x}_c^{\phi}(t)$ and $\mathbf{H}(t)$ with $\mathbf{H}^{\phi}(t)$. Therefore, we infer that $\lambda_{min}(\mathbf{H}^{\phi}(t))$ *of any convolutional layer is positively correlated with the convergence and generalisation of a CNN.*

Additionally, the eigenvalues of $\mathbf{H}^{\phi}(t)$ represent the variance along the orthogonal eigenvectors. These eigenvectors capture the orthogonal directions of the variability of the data (Shawe-Taylor et al., 2005). Consequently, $\lambda_{min}(\mathbf{H}^{\phi}(t))$ *shows the uniqueness of information in the most linearly dependent channel or feature map in* $\mathbf{X}^{\phi}(t)$. Lower values of $\lambda_{min}(\mathbf{H}^{\phi}(t))$ indicate that at least one channel in $\mathbf{X}^{\phi}(t)$ is highly redundant and could be represented as a linear combination of other channels.

Instead of focusing solely on the linear dependence or collinearity of the most linearly dependent channel in $\mathbf{X}^{\phi}(t)$, we focus on the collinearity among all channels jointly. Thus, we assume that the convergence and generalisation of f_{cnn} are negatively correlated to the multi-collinearity of channels in $\mathbf{X}^{\phi}(t)$. This assumption is proved later in Theorems 3 and 4.

3.3.2 Singular Value Decomposition for multi-collinearity

To estimate the multi-collinearity in $\mathbf{X}^{\phi}(t)$, we deploy SVD due to its effectiveness and numerical stability, especially when considering large ill-conditioned matrices (Klema & Laub, 1980). We know that the singular values σ_k of $\mathbf{X}^{\phi}(t)$ are equal to the square root of the eigenvalues λ_k of the gram matrix $\mathbf{H}^{\phi}(t)$ at any time-step t, i.e. $\sigma_k = \sqrt{\lambda_k(\mathbf{H}^{\phi}(t))}$, where k indexes the orthogonal eigenvectors.

Remark 4 *The condition number of* $\mathbf{X}^{\phi}(t)$*, defined as the ratio of the maximum singular value to the minimum singular value, i.e.* $c(\mathbf{X}^{\phi}(t)) = \sigma_{max}(\mathbf{X}^{\phi}(t))/\sigma_{min}(\mathbf{X}^{\phi}(t)) \in \mathbb{R}$*, calculated through SVD, depicts the ill-conditioning or collinearity of vectors in* $\mathbf{X}^{\phi}(t)$ *(Demmel, 1987).*

Thus, we utilise the condition number $c(\mathbf{X}^{\phi}(t))$ to establish the relationship between the collinearity of channels in $\mathbf{X}^{\phi}(t)$ and the convergence and generalisation properties of the CNN f_{cnn}. Hence, we present the following assumption and theorems concerning convergence and generalisation through adaptation of the theorems presented in Section 3.2.1.

Assumption 1 *Consider a multi-channel convolutional layer with the number of channels as* C*, then the maximum singular value of* $\mathbf{X}^{\phi}(t)$ *is greater than or equal to 1, i.e.* $\sigma_{max}(\mathbf{X}^{\phi}(t)) \geq 1$*. The proof and the experimental validation is provided in the Appendix Sections A.1.3 and A.1.4 respectively.*

Theorem 3 *Consider a multi-channel convolutional neural network* f_{cnn} *that is approximated by the network* f*. Let the input to* f *be* $i \in [n]$ *and* $c_{low} < ||\mathbf{x}_i||_2 < c_{high}$*,* $|y_i| < C$ *for some constant* c_{low}*,* c_{high}*, and* C*. Next, consider the Assumption 1 to be satisfied, and that the number of nodes* m *for* f *is selected according to* $\Omega(\frac{n^6}{\lambda_{min}(\mathbf{H}^{\infty})^4\delta^6})$*, where* Ω *represents the lower bound. Then, if we perform an i.i.d. initialisation of* $\mathbf{w}_r \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ *and let* $a_r \sim \mathcal{U}\{[-1, 1]\}$ *for* $r \in [m]$*, where* $\mathcal{U}$ *denotes a uniform distribution, then with a probability of at least* $1 - \delta$*, the following inequality holds for* f_{cnn}*:*

$$\|\mathbf{u}_i^{\phi}(t) - \mathbf{y}_i\|_2^2 \leq \exp(-t/c(\mathbf{X}_i^{\phi}(t=0))^2)\|\mathbf{u}_i^{\phi}(0) - \mathbf{y}_i\|_2^2, \tag{6}$$

where $\mathbf{X}_i^{\phi}(t=0)$ *is the scaled feature matrix at initialisation, i.e.* $t = 0$*.*

We observe from Theorem 3 that $c(\mathbf{X}^{\phi}(t=0))^2$ *negatively correlates with the convergence rate.* Thus, through Remark 4 and Theorem 3, we deduce that the convergence rate worsens with the increase in multi-collinearity of $\mathbf{X}^{\phi}(t=0)$. The proof for Theorem 3 is available in the Appendix Section A.1.

Table 1: Comparison of Spearman rank correlation coefficient for various zero-cost proxies on four tasks of TransNASBench101-micro (TNB), along with NAS-Bench-101 (NB101), NAS-Bench-201 (NB201), and NAS-Bench-301 (NB301). We report the mean and standard deviation of our results across 3 runs. The best approach is indicated as **bold** and the second-best approach is indicated as underlined. All numbers except ours and MeCo (Jiang et al., 2023) are taken from (Peng et al., 2024).

Approach	TNB-Object	TNB-Scene	TNB-Jigsaw	NB101	NB201-cf10	NB201-cf100	NB201-ImNet120	NB301
Grasp	-0.22	-0.43	-0.12	0.27	0.39	0.46	0.45	0.34
Fisher	0.44	-0.13	0.30	-0.28	0.40	0.46	0.42	-0.28
Grad_Norm	0.39	-0.33	0.36	-0.24	0.42	0.49	0.47	-0.04
Snip	0.45	-0.14	0.41	-0.19	0.43	0.49	0.48	-0.05
Synflow	0.48	0.27	0.47	0.31	0.74	0.76	0.75	0.18
#params	0.45	0.32	0.44	0.38	0.72	0.73	0.69	0.46
ZiCo	0.50	0.70	0.52	$0.41^{\dagger}$	0.76	0.79	0.77	$\mathbf{0.49}^{\dagger}$
MeCo	**0.58**	0.62	0.45	$0.57^{\dagger}$	0.89	0.88	0.85	$0.43^{\dagger}$
Swap_reg	0.48	0.67	0.47	$0.49^{\dagger}$	0.88	0.90	**0.87**	$\mathbf{0.49}^{\dagger}$
Dextr (ours)	0.53±0.007	**0.75±0.003**	**0.55±0.003**	**0.65±0.010**	**0.90±0.006**	**0.91±0.004**	**0.87±0.006**	0.44±0.007

Theorem 4 *For the test loss function $L^{\phi}(\mathbf{W})$ of the network f_{cnn}, let the SGD step-size γ be determined by $\gamma = kC_1\sqrt{\mathbf{y}^T(\mathbf{H}^{\infty})^{-1}\mathbf{y}}/(m\sqrt{N})$, where k is a small absolute constant. Let the ground truth $\mathbf{y} = (y_1, ..., y_N)^T$, where N is the number of samples. If Theorem 3 holds, then for any $\delta \in (0, e^{-1}]$, there exists a value m^* which depends on δ, N, and $c(\mathbf{X}^{\phi}(t=0))$ such that if $m \geq m^*$, then with a probability of at least $1-\delta$, the following inequality holds:*

$$\mathbb{E}[L^{\phi}(\mathbf{W})] \leq \mathcal{O}\left(C_2 c(\mathbf{X}^{\phi}(t=0))\sqrt{\frac{\mathbf{y}^T\mathbf{y}}{N}}\right) + \mathcal{O}\left(\sqrt{\frac{\log(1/\delta)}{N}}\right), \tag{7}$$

where C_1 and C_2 are constants.

The proof for this theorem is presented in the Appendix Section A.1. We observe from Theorem 3 that the upper bound of the test loss of f_{cnn} is directly proportional to $c(\mathbf{X}^{\phi}(t=0))$. Hence, $c(\mathbf{X}^{\phi}(t=0))$ is inversely proportional to the generalisation capabilities of f_{cnn}.

We now see from Theorem 3 and 4 that *the convergence and generalisation of f_{cnn} are negatively correlated to the multi-collinearity of feature maps of a given layer at initialisation*, which is also observed in Figure 1b. Next, we formulate Dextr through the proposed theorems.

3.3.3 Formulating Dextr

Through the Theorem 3 and 4, we note that $c(\mathbf{X}^{\phi}(t=0))$ correlates negatively with the convergence and generalisation of f_{cnn}. Through Remark 1, we know that $\mathbf{H}(t)$ stays close to $\mathbf{H}^{\infty}$ (when $t=0$) if $m \to \infty$. Hence, we infer that $\lambda_{min}(\mathbf{H}^{\phi}(t))$ approximates the value of $\lambda_{min}(\mathbf{H}^{\phi}(t=0))$. Thus, through the relation $\sigma_k = \sqrt{\lambda_k(\mathbf{H}^{\phi}(t))}$, we know that the condition number $c(\mathbf{X}^{\phi}(t))$ also approximates the value $c(\mathbf{X}^{\phi}(t=0))$. Hence, *the inverse of $c(\mathbf{X}^{\phi}(t))$ correlates positively with the convergence and generalisation.* Subsequently, through Remark 2, we observe that *the extrinsic curvature of the output, i.e. $\kappa(\theta)$ correlates positively with the expressivity characteristics of f_{cnn}.* To balance convergence, generalisation, and expressivity characterisations, we propose the following zero-cost proxy using the simplified harmonic mean of the logarithms of the extrinsic curvature $\kappa(\theta)$ and the sum of the inverse of the feature condition number $c(\mathbf{X}^{\phi}(t))$:

$$Dextr = \frac{\log\left(1 + \sum_{l=1}^{L} \frac{1}{c_l(\mathbf{X}^{\phi})}\right) \cdot \log\left(1 + \kappa(\theta)\right)}{\log\left(1 + \sum_{l=1}^{L} \frac{1}{c_l(\mathbf{X}^{\phi})}\right) + \log\left(1 + \kappa(\theta)\right)} \tag{8}$$

where L is the number of layers, $c_l(\mathbf{X}^{\phi})$ is the condition number corresponding to the feature maps of layer l and $\kappa(\theta)$ is the extrinsic curvature of the output given an arbitrary circular input θ. As observed from Eq. 8, the proposed proxy is defined as the half of the harmonic mean between two terms: $\log\left(1 + \sum_{l=1}^{L} \frac{1}{c_l(\mathbf{X}^{\phi})}\right)$ and $\log\left(1 + \kappa(\theta)\right)$. The logarithmic transformations in Eq. 8 are applied to reduce the effect of the scale of

these two terms and to avoid numerical instabilities, while the addition of 1 ensures that both terms remain positive. Note that we omit the training time step t in our proposed proxy as Dextr is invariant to t, meaning theoretically, feature maps $\mathbf{X}^{\phi}$ and curvature $\kappa(\theta)$ at any point in training can be used to calculate Dextr.*

3.3.4 Application to Vision Transformers

To demonstrate the application of Dextr to Vision Transformers (ViTs) (Dosovitskiy et al., 2021), we rely on the relation of CNNs with ViTs given by Li et al. (2021a). Notably, Li et al. (2021a) prove that a multi-head self-attention (MSA) layer in ViTs with relative positional encoding can exactly mimic a convolution operation if the number of heads is carefully set with a sufficient number, mainly due to the similarities between the attention mechanism and convolutions. This supports the applicability of our convolutional layer analysis (Section 3.2.3) to ViTs. Lastly, we consider the Gaussian Error Linear Units (GeLU) activation function (Hendrycks & Gimpel, 2016) used in ViTs. Since GeLU is regarded as a smooth approximation of ReLU (Hendrycks & Gimpel, 2016), the behaviour of these functions is comparable. Thus, the concepts discussed earlier in relation to ReLUs can be directly applied to GeLUs as well.

4 Experiments

Our evaluation is performed through two standard protocols (Li et al., 2023; Jiang et al., 2023; Sun et al., 2023), namely the correlation experiments and NAS experiments. The experiments include a total of six benchmarks involving CNN and ViT architectures. We evaluate our method on a variety of supervised and self-supervised tasks, including image classification (Ying et al., 2019; Dong & Yang, 2020; Zela et al., 2022), object classification (Duan et al., 2021), scene classification (Duan et al., 2021), and jigsaw classification (Duan et al., 2021).

4.1 Experimental Protocol

Correlation experiments We first consider the correlation experiments. To this end, we evaluate our proposed zero-cost proxy on four standard benchmarks: NAS-Bench-101 (Ying et al., 2019), NAS-Bench-201 (Dong & Yang, 2020), NAS-Bench-301 (Zela et al., 2022), and TransNAS-Bench-101-micro (Duan et al., 2021) through the NAS-Bench-Suite-Zero framework (Krishnakumar et al., 2022) for an unbiased comparison (Peng et al., 2024). Additionaly, we provide correlation experiments on NATS-Bench-SSS (Dong et al., 2021) in the Appendix Section A.3. To evaluate our approach, we utilise the standard evaluation protocol (Peng et al., 2024; Jiang et al., 2023; Li et al., 2023), calculating the Spearman rank correlation coefficient (Zar, 2005) between the proxy value and the architecture test accuracy. We consider 1000 randomly sampled architectures from NAS-Bench-Suite-Zero for our analysis. We perform 3 runs of each correlation experiment and compare the mean proxy-accuracy correlation of Dextr with several zero-cost proxies, following the same evaluation protocol, namely Fisher (Turner et al., 2020), Snip (Lee et al., 2019), Grasp (Wang et al., 2020), Synflow (Tanaka et al., 2020), Grad_Norm (Abdelfattah et al., 2021), MeCo (Jiang et al., 2023), SWAP-NAS (Peng et al., 2024), and the number of parameters #params.

NAS experiments Our NAS experiments involve searching architectures for the ImageNet (Deng et al., 2009) classification task and comprise two search spaces- AutoFormer (Chen et al., 2021b) search space containing Vision Transformer (ViT) architectures and DARTS search space containing CNNs (Liu et al., 2019). We conduct an additional experiment on MobileNet-v2 space (Sandler et al., 2018), available in the Appendix Section A.3.2.

Our DARTS evaluation follows the standard protocol (Liu et al., 2019; Chen et al., 2021c; Peng et al., 2022) of searching for the optimal architecture on CIFAR-10 and training the found architecture on ImageNet (Deng et al., 2009). Furthermore, the search for the best architecture for all zero-cost proxies is based on the operation scoring strategy through the Zero-Cost-PT algorithm (Xiang et al., 2023). We perform the search

*We provide the procedure to calculate Dextr and the experimental settings in the Appendix Sections A.4 and A.5 respectively.

†Experiments marked by † are rerun through their official implementation using the NAS-Bench-Suite Zero (Krishnakumar et al., 2022) framework.

Table 2: Quantitative comparison of networks chosen by the NAS methods on ImageNet (Deng et al., 2009) within the DARTS (Liu et al., 2019) search space in terms of the top-1 and top-5 error rate, along with the number of parameters (Params), Method Type (One Shot, Zero-Shot, or Predictor) and search cost in GPU days. The best approach is indicated as **bold** and the second-best approach is indicated as underlined.

Method	Top-1/Top-5 ↓ Error	Params (M)	GPU Days ↓	Type
DARTS (2nd) (Liu et al., 2019)	26.7 / 8.7	4.7	4.0	OS
SNAS (Xie et al., 2018)	27.3/9.2	4.3	1.5	OS
FairDARTS (Chu et al., 2020b)	24.4/7.4	5.3	3.8	OS
PC-DARTS (Xu et al., 2019)	25.1/ 7.8	5.3	0.1	OS
P-DARTS (Chen et al., 2019)	24.4 / 7.4	4.9	0.3	OS
β-DARTS (Ye et al., 2022)	**23.9 / 7.0**	5.5	0.4	OS
PRE-NAS (Peng et al., 2022)	24.0/7.8	6.2	0.6	PR
TE-NAS (Chen et al., 2021c)	26.2 / 8.3	6.3	0.05	ZS
ZiCo [3] (Li et al., 2023)	24.9/7.6	7.7	0.02	ZS
MeCo [3] (Jiang et al., 2023)	25.1/7.7	7.8	0.04	ZS
Dextr (ours)	**24.6/7.4**	6.6	0.07	ZS

Table 3: Quantitative comparison for the AutoFormer (Chen et al., 2021b) search space in the Tiny and Small setting with parameter constraints 6M and 24M respectively. We report the top-1 error, the number of parameters (Params) and floating point operations (FLOPs) of selected networks on ImageNet (Deng et al., 2009), along with the search cost in GPU days. The best approach is indicated as **bold** and the second-best approach is indicated as underlined.

Method	Top-1 Error ↓	Params (M)	FLOPs	GPU Days ↓
Tiny (6M)				
AutoFormer (Chen et al., 2021b)	25.3	5.7	1.30G	24
AZ-NAS (Lee & Ham, 2024)	23.9	5.9	1.38G	0.03
Dextr (ours)	**23.7**	5.8	1.36G	0.03
Small (24M)				
AutoFormer (Chen et al., 2021b)	18.3	22.9	5.10G	24
TF-TAS (Zhou et al., 2022)	18.1	23.9	5.16G	0.5
AZ-NAS (Lee & Ham, 2024)	**17.8**	23.8	5.13G	0.07
Dextr (ours)	18.0	23.0	4.93G	0.07

and training procedures and report the top-1 and top-5 error of the architecture found by Dextr, along with the number of parameters and search cost in GPU days, and compare with various baseline one-shot and zero-shot NAS approaches, including DARTS (Liu et al., 2019), SNAS (Xie et al., 2018), FairDARTS (Chu et al., 2020b), PC-DARTS (Xu et al., 2019), P-DARTS (Chen et al., 2019), β-DARTS (Ye et al., 2022), PRE-NAS (Peng et al., 2022), TE-NAS (Chen et al., 2021c), MeCo (Jiang et al., 2023), and ZiCo (Li et al., 2023).

Next, we consider our evaluation in the AutoFormer search space (Chen et al., 2021b). The AutoFormer (Chen et al., 2021b) search space is segregated into three subspaces- tiny, small and base with varying architecture sizes. In our experiments, we consider the tiny and small subspaces of AutoFormer to leverage faster training times. We follow the standard protocol (Chen et al., 2021b; Zhou et al., 2022; Lee & Ham, 2024) which involves searching for the parameter-constrained architecture with the best Dextr score among 1000 candidate architectures. The selected ViT is then trained on ImageNet with an identical experimental setup as (Zhou et al., 2022; Lee & Ham, 2024). Our approach is compared with several baselines, namely AutoFormer (Chen et al., 2021b), TF-TAS (Zhou et al., 2022), and AZ-NAS (Lee & Ham, 2024). We compare the top-1 error, number of parameters (Params), number of floating point operations (FLOPs) and search cost of the architecture in GPU days found through our method with the baselines.

4.2 Discussion of Results

Correlation results Table 1 presents the comparison of Spearman rank correlation coefficient ρ across different zero-cost proxies. Our method consistently surpasses previous baselines across the NAS-Bench-101 and NAS-Bench-201, and in two out of three tasks of TransNAS-Bench-101-micro benchmark. Remarkably, in the case of NAS-Bench-101, our approach shows an improvement of 8% over the previous best approach. In the NAS-Bench-301 benchmark, our method performs competitively with a correlation of 44%. Notably, our approach demonstrates superior performance in both supervised tasks (scene classification) and self-supervised tasks (jigsaw classification), highlighting its versatility and effectiveness across a range of computer vision tasks. Lastly, as evident from the low standard deviation values, we observe that the results of our approach are stable across different runs.

NAS results Our NAS experiments on DARTS and AutoFormer search spaces are summarised in Table 2 and 3 respectively. Table 2 shows that our proposed approach efficiently searches for architectures with low test errors on ImageNet, completing the search in only 0.07 GPU days. Specifically, Dextr achieves lower error rates and is faster compared to previous one-shot methods, such as DARTS (Liu et al., 2019), SNAS (Xie et al., 2018), and PC-DARTS (Xu et al., 2019), while relying on only a single label-free data sample. Furthermore, Dextr demonstrates superior performance over all prior state-of-the-art zero-shot methods with a comparable search cost. Although some one-shot approaches like FairDARTS (Chu et al., 2020b), P-DARTS (Chen et al., 2019), β-DARTS (Ye et al., 2022), and PRE-NAS (Peng et al., 2022) achieve better test error, our approach is at least approximately 2.3x faster than any of these approaches with marginal difference in test error.

Moreover, we observe from Table 3 that our approach outperforms the previous best methods in the AutoFormer-tiny search space and demonstrates competitive performance in the AutoFormer- small search space in terms of Top-1 error while being at least as fast as the previous fastest approach.

4.3 Ablation Studies

4.3.1 Stability of Dextr

In this study, we assess the stability of our approach. To this end, we sample 10 architectures from NAS-Bench-201 (Dong & Yang, 2020) search space. Next, for each network, we calculate 10 Dextr values corresponding to 10 random inputs taken from CIFAR-10, along with randomly generated circular inputs $\mathbf{g}(\theta)$ for our curvature calculation. Finally, we calculate the mean and standard deviation of the different Dextr values of each network and report them in Table 4, along with the test accuracy of that network.

Table 4: Mean and Standard Deviation of Dextr for 10 networks sampled from NAS-Bench-201 (Dong & Yang, 2020), corresponding to 10 random inputs taken from CIFAR-10 and 10 randomly generated circular inputs $\mathbf{g}(\theta)$. StD. denotes the Standard Deviation and Acc. denotes the test accuracy of the network.

Network	Mean	StD.	Acc. (%)
1	1.39	0.03	81.52
2	2.11	0.07	90.51
3	1.56	0.07	81.84
4	1.52	0.04	83.88
5	1.49	0.04	84.49
6	1.77	0.05	87.78
7	2.10	0.06	88.65
8	1.90	0.06	88.77
9	1.88	0.08	88.81
10	1.50	0.04	84.12

We observe from Table 4 that our approach is stable with different randomly sampled inputs and different circular inputs (used in the calculation of curvature), which is proved by low standard deviation values in

Table 5: Quantitative comparison of spearman rank correlation coefficient ρ between Dextr and a harmonic mean of Zen and ZiCo on NAS-Bench-201 (Dong & Yang, 2020).

Method	CIFAR-10	CIFAR-100	ImageNet16-120
HM (Zen,ZiCo)	0.44	0.44	0.47
Dextr (ours)	**0.90**	**0.91**	**0.87**

the results. Moreover, we observe the expected behaviour that the network with the lowest mean exhibits the lowest test accuracy while the highest mean corresponds to the best performing network.

4.3.2 Comparison with a simple combination of existing proxies

We now compare the Spearman rank correlation coefficient ρ of the harmonic mean of two existing proxies, focused on convergence, generalisation, and expressivity. Specifically, we compare Dextr with the harmonic mean of Zen (Lin et al., 2021) (expressivity) and ZiCo (Li et al., 2023) (convergence, generalisation) on NAS-Bench-201 in Table 5. We observe that Dextr significantly outperforms the simple combination of proxies focused on individual attributes, thus proving the effectiveness of the proposed specific combination.

4.3.3 Analysis for individual layers

We study the variation in linear independence of feature maps (FMI) across different hidden layers of networks sampled from NAS-Bench-201 (Dong & Yang, 2020). The FMI is calculated using the inverse of the condition number, i.e. $1/c(\mathbf{X}^{\phi})$. We compare the FMI between layers of a high-performing network, with a validation accuracy of 89.43% and a low-performing network, with a validation accuracy of 63%. The results, shown in Figure 2, reveal that the FMI of the networks fluctuates due to considering outputs from all layers, including activations, convolutions, and fully connected layers. Peaks in FMI increase, then slightly decrease, and finally drop to zero, with the highest peaks occurring during network dimensionality expansion. Finally, the low-performing network's layer outputs are generally less linearly independent, supporting the theoretical findings in Theorems 3 and 4.

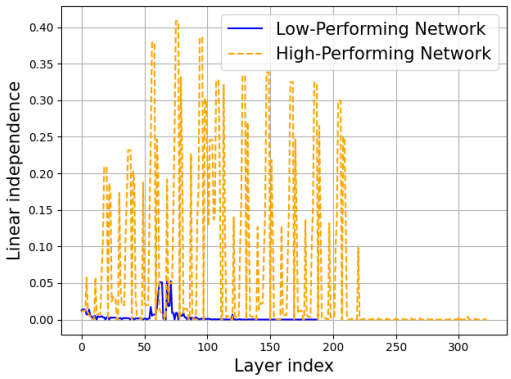


Figure 2: Graph depicting the linear independence of outputs, calculated using $1/c(\mathbf{X}^{\phi})$, for each hidden layer of two CNNs. We observe that the hidden layer outputs of the high-performing network are more linearly independent than the low-performing network.

5 Conclusion

We presented a zero-cost proxy, Dextr. To this end, we first demonstrated the relationship between the collinearity of the features and the convergence and generalisation of a network through SVD. Next, we exploited concepts from Riemannian geometry to include expressivity in our proxy. Our experiments demonstrated that our proxy exhibits a strong correlation with network performance without requiring labelled data. As a result, it outperforms all previous proxies in NAS-Bench-101, NAS-Bench-201, and TransNAS-Bench-micro benchmarks, along with established multi-shot and zero-shot NAS baselines in the ImageNet experiment in the DARTS and AutoFormer search space, all while inducing a low search cost.

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A Appendix

A.1 Proofs and Derviations

A.1.1 Proof for Theorem 3

We start from Theorem 1, which states:

Theorem 1 *Let the input be $i \in [n]$, $c_{low} < \|\mathbf{x}_i\|_2 < c_{high}$ and $\|y_i\| < C$, where C is a constant. If the number of nodes m is set to $\Omega(\frac{n^6}{\lambda_{min}(\mathbf{H}^\infty)^4\delta^6})$, where δ is the probability of failure, Ω denotes the lower bound, and $\lambda_{min}(\mathbf{H}^\infty)$ denotes the scaled minimum eigenvalue of $\mathbf{H}^\infty$, and we i.i.d. initialise $\mathbf{w}_r \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and $a_r \sim \mathcal{U}\{[-1, 1]\}$, where $\mathcal{U}\{\cdot\}$ represents the uniform distribution, then with at least $1 - \delta$ probability, the following relationship holds,*

$$\|\mathbf{u}_i(t) - \mathbf{y}_i\|_2^2 \leq \exp(-\lambda_{min}(\mathbf{H}^\infty)t)\|\mathbf{u}_i(0) - \mathbf{y}_i\|_2^2. \tag{9}$$

By relying on Assumption 1, we know that $\sigma_{max}(\mathbf{X}^\phi(t = 0)) \geq 1$ and thus, $\lambda_{\max}(\mathbf{H}^\infty) \geq 1$. Hence, we divide the term $\lambda_{min}(\mathbf{H}^\infty)t$ with $\lambda_{\max}(\mathbf{H}^\infty)$ and obtain the following inequality

$$\|\mathbf{u}_i(t) - \mathbf{y}_i\|_2^2 \leq \exp\left(-\frac{\lambda_{\min}(\mathbf{H}^\infty)}{\lambda_{\max}(\mathbf{H}^\infty)}t\right)\|\mathbf{u}_i(0) - \mathbf{y}_i\|_2^2. \tag{10}$$

This inequality holds because $\lambda_{\max}(\mathbf{H}^\infty) \geq 1$ implies that $\frac{\lambda_{\min}(\mathbf{H}^\infty)}{\lambda_{\max}(\mathbf{H}^\infty)} \leq \lambda_{\min}(\mathbf{H}^\infty)$, and the exponential function with negative exponent is monotonically decreasing.

Next, we use Remark 3 to approximate the gram matrix concerning the fully connected layer of f, i.e. $\mathbf{H}^\infty$ with the gram matrix of the convolutional layer of the CNN f_{cnn} $\mathbf{H}^\phi(t = 0)$. This allows us to re-parameterize the eigenvalues λ_k of $\mathbf{H}^\infty$ into singular values $\sigma_k(\mathbf{X}^\phi(t = 0))$ using the equation $\sigma_k(\mathbf{X}^\phi(t)) = \sqrt{\lambda_k(\mathbf{H}^\phi(t))}$. Then, by replacing the network output of f, i.e. $\mathbf{u}_i(t)$ with the network output of f_{cnn}, i.e. $\mathbf{u}_i^\phi(t)$, we obtain

$$\begin{aligned}\|\mathbf{u}_i^\phi(t) - \mathbf{y}_i\|_2^2 &\leq \exp\left(-\left(\frac{\sigma_{\min}(\mathbf{X}^\phi(0))}{\sigma_{\max}(\mathbf{X}^\phi(0))}\right)^2 t\right)\|\mathbf{u}_i^\phi(0) - \mathbf{y}_i\|_2^2 \\ &\leq \exp\left(-\frac{t}{c\left(\sigma_{\max}(\mathbf{X}^\phi(0))\right)^2}\right)\|\mathbf{u}_i^\phi(0) - \mathbf{y}_i\|_2^2.\end{aligned} \tag{11}$$

which completes the proof.

A.1.2 Proof for Theorem 4

We start from from Theorem 2, which states

Theorem 2 *Let the loss function of f with $m \to \infty$ evaluated on the test set be denoted as $L(\mathbf{W})$. Let the ground truth $\mathbf{y} = (y_1, ..., y_N)^T$, and γ represent the step size of stochastic gradient descent (SGD), determined by $\gamma = kC_1\sqrt{\mathbf{y}^T(\mathbf{H}^\infty)^{-1}\mathbf{y}}/(m\sqrt{N})$, where k is a sufficiently small absolute constant. If Theorem 1 holds, then for any $\delta \in (0, e^{-1}]$, there exists a value m^* which depends on $\delta, N, \lambda_{min}(\mathbf{H}^\infty$ such that if $m \geq m^*$, with a probability of at least $1 - \delta$, the following inequality holds:*

$$\mathbb{E}[L(\mathbf{W})] \leq \mathcal{O}\left(C_2\sqrt{\frac{\mathbf{y}^T\mathbf{y}}{\lambda_{min}(\mathbf{H}^\infty)N}}\right) + \mathcal{O}\left(\sqrt{\frac{\log(1/\delta)}{N}}\right) \tag{12}$$

, where C_1 and C_2 are constants.

Using Assumption 1, we know that $|\sigma_{max}(\mathbf{X}^\phi(t = 0))| \geq 1$ and thus, $\lambda_{\max}(\mathbf{H}^\infty) \geq 1$. Thus, we can derive the following inequality:

$$\mathbb{E}[L(\mathbf{W})] \leq \mathcal{O}\left(C_2\sqrt{\frac{\lambda_{\max}(\mathbf{H}^{\infty})}{\lambda_{\min}(\mathbf{H}^{\infty})}}\sqrt{\frac{\mathbf{y}^T\mathbf{y}}{N}}\right) \tag{13}$$

$$+\mathcal{O}\left(\sqrt{\frac{\log(1/\delta)}{N}}\right) \tag{14}$$

Next, we use Remark 3 to approximate the gram matrix of a fully connected layer $\mathbf{H}^{\infty}$ with a convolution layer $\mathbf{H}^{\phi}(t=0)$. This allows us to re-parameterize the eigenvalues $\lambda_k(\mathbf{H}^{\infty})$ into singular values $\sigma_k(\mathbf{X}^{\phi}(t=0))$ using the equation $\sigma_k(\mathbf{X}^{\phi}(t=0)) = \sqrt{\lambda_k \mathbf{H}^{\phi}(t=0)}$. By replacing the loss term $\mathbb{E}[L(\mathbf{W})]$ with the CNN loss term $\mathbb{E}[L^{\phi}(\mathbf{W})]$, we obtain

$$\begin{aligned}\mathbb{E}[L^{\phi}(\mathbf{W})] &\leq \mathcal{O}\left(C_2\frac{\sigma_{\max}(\mathbf{X}^{\phi}(0))}{\sigma_{\min}(\mathbf{X}^{\phi}(0))}\sqrt{\frac{\mathbf{y}^T\mathbf{y}}{N}}\right)\\ &+\mathcal{O}\left(\sqrt{\frac{\log(1/\delta)}{N}}\right)\\ &\leq \mathcal{O}\left(C_2 c(\mathbf{X}^{\phi}(0))\sqrt{\frac{\mathbf{y}^T\mathbf{y}}{N}}\right)\\ &+\mathcal{O}\left(\sqrt{\frac{\log(1/\delta)}{N}}\right).\end{aligned} \tag{15}$$

which completes the proof.

A.1.3 Proof for Assumption 1

Let $x_{\hat{i}\hat{j}}$ denote the $\hat{i}\hat{j}$-th entry of $\mathbf{X}^{\phi}(t)$. We know from the Courant–Fischer–Weyl Min-Max-theorem (Il'yasov & Muravnik, 2022) that $\sigma_{max}(\mathbf{X}^{\phi}(t)) = \max_{\|u\|=1} \|\mathbf{X}^{\phi}(t)u\|)$ or any unit vector u. Then, we obtain

$$\sigma_{max}(\mathbf{X}^{\phi}(t) \geq \sqrt{\sum_{i=1}^{C} x_{\hat{i}\hat{j}}^2} \tag{16}$$

$$\geq \sqrt{x_{\hat{i}\hat{j}}^2} \tag{17}$$

$$\geq |x_{\hat{i}\hat{j}}| \forall \hat{i}, \hat{j} \tag{18}$$

, which shows that the maximum singular value of $\mathbf{X}^{\phi}(t)$ is larger than the maximum value in the matrix $\mathbf{X}^{\phi}(t)$. Next, we assume that at least one absolute entry in the output induced by the ReLU activation function is greater than 1, i.e. $|x_{\hat{i}\hat{j}}| \geq 1 \exists \hat{i}, \hat{j}$. Thus, the assumption $\sigma_{max}(\mathbf{X}^{\phi}(t)) \geq 1$ holds true in general, which is further validated in Section A.1.4.

A.1.4 Experimental validation for Assumption 1

To provide experimental validation for Assumption 1, we conduct an analysis examining the number of cases where our assumption holds true, i.e. where $\sigma_{max}(\mathbf{X}^{\phi}(t)) \geq 1$. To this end, we sample 1000 networks from NAS-Bench-101 (Ying et al., 2019), NAS-Bench-201 (Dong & Yang, 2020), and NAS-Bench-301 (Zela et al., 2022) through the NAS-Bench-Suite-Zero (Krishnakumar et al., 2022) framework. Next, we input a random data sample from CIFAR-10 to each of these networks and calculate the mean of the percentage of layers

Table 6: The mean percentage of layers corresponding to 1000 networks in three different benchmarks where Assumption 1 holds true, i.e. $\sigma_{max}(\mathbf{X}^{\phi}(t)) \geq 1$.

Benchmark	$\sigma_{max}(\mathbf{X}^{\phi}(t)) \geq 1$
NAS-Bench-101	99.18 %
NAS-Bench-201	90.01 %
NAS-Bench-301	99.51 %

Table 7: Comparison of the Spearman rank correlation coefficient on NATS-Bench-SSS (Dong et al., 2021) across different datasets for various zero-cost proxies.

Methods	CIFAR-10	CIFAR-100	ImageNet16-120
#params	0.72	0.73	0.84
Fisher (Turner et al., 2020)	0.44	0.55	0.47
Snip (Lee et al., 2019)	0.59	0.62	0.76
Grasp (Wang et al., 2020)	-0.13	0.01	0.42
Synflow (Tanaka et al., 2020)	0.81	0.80	0.57
Grad_Norm (Abdelfattah et al., 2021)	0.51	0.49	0.67
NTK (Chen et al., 2021c)	0.34	0.29	0.28
Zen (Lin et al., 2021)	0.69	0.71	0.87
ZiCo (Li et al., 2023)	0.73	0.75	0.88
MeCo (Jiang et al., 2023)	-0.79	-0.87	-0.86
Dextr (ours)	-0.63 $\pm$ 0.006	-0.60 $\pm$ 0.005	-0.67 $\pm$ 0.006

where $\sigma_{max}(\mathbf{X}^{\phi}(t)) \geq 1$. From Table 6, we observe that for all the benchmarks for at least 90% of the cases, $\sigma_{max}(\mathbf{X}^{\phi}(t)) \geq 1$. Remarkably, in NAS-Bench-101 and NAS-Bench-301, Assumption 1 holds true for almost all the layer outputs.

A.2 Additional Experiments

A.3 NATS-Bench-SSS

We now conduct correlation experiments on the NATS-Bench-SSS (Dong et al., 2021) benchmark. The NATS-Bench-SSS benchmark is fundamentally different from other correlation benchmarks (Dong & Yang, 2020; Ying et al., 2019; Zela et al., 2022), as it contains architectures of varying numbers of channels. We follow the same evaluation protocol as the other correlation experiments, detailed in Section 4.1 of the main paper. We report the mean Spearman Rank Correlation Coefficient ρ and standard deviation, averaged over 3 runs of Dextr in Table 7 and compare it with various baselines.

We observe from the results that in unlike other benchmarks, our approach exhibits a negative correlation weaker than some of the previous methods in the NATS-Bench-SSS benchmark. Upon investigating, we found out that this discrepancy arises due to the sensitivity of the condition number $c(\mathbf{X})$ to the number of channels, similarly exhibited by MeCo (Jiang et al., 2023). This behaviour is specific to the NATS-Bench-SSS benchmark as it contains architectures of varying number of channels. We rectify this behaviour for this benchmark through the optimisation procedure detailed in the Section A.3.1.

A.3.1 Dextr optimisation

As observed in the NATS-Bench-SSS (Dong et al., 2021) correlation experiment detailed in Table 7, Dextr achieves a negative correlation with the accuracy of the architecture. We utilise the optimisation procedure detailed by (Jiang et al., 2023) to fix this discrepancy. Specifically, instead of considering all the channels of the network layer, we randomly sample a fixed number of channels and calculate the Dextr value using the formula

Table 8: Comparison of the Spearman rank correlation coefficient between Dextr and the optimised version of Dextr (Dextr_{opt}) on NATS-Bench-SSS (Dong et al., 2021).

Methods	CIFAR-10	CIFAR-100	ImageNet16-120
Dextr	**-0.63**	-0.60	**-0.67**
Dextr_{opt}	0.56	**0.66**	0.65

Table 9: Quantitative comparison for the MobileNet-v2 (Sandler et al., 2018) search space with FLOPs constraint of 450M. We report the top-1 accuracy, floating point operations (FLOPs) of selected networks on ImageNet (Deng et al., 2009), the type of search method- multi-shot (MS), one-shot (OS) or zero-shot (ZS), along with the search cost in GPU days. The best approach is indicated as **bold** and the second-best approach is indicated as underlined.

Method	FLOPs (M)	Top-1 Acc. (%) ↑	Type	Search Cost (GPU Days)↓
NAS-Net-B (Zoph et al., 2018)	488	72.8	MS	1800
CARS-D (Yang et al., 2020b)	496	73.3	MS	0.4
BN-NAS (Chen et al., 2021a)	470	75.7	MS	0.8
OFA (Cai et al.)	406	77.7	OS	50
RLNAS (Zhang et al., 2021)	473	75.6	OS	-
DONNA (Moons et al., 2021)	501	78.0	OS	405
#params	451	63.5	ZS	0.02
ZiCo (Li et al., 2023)	448	78.1	ZS	0.4
AZ-NAS (Lee & Ham, 2024)	462	78.6	ZS	0.4
Dextr (ours)	457	**78.8**	ZS	0.6

$$\text{Dextr}_{opt} = \frac{\log\left(1 + \sum_{l=1}^{L} \frac{\alpha_l}{\beta c_l(\mathbf{X}^{\phi'})}\right) \cdot \log(1 + \kappa(\theta))}{\log\left(1 + \sum_{l=1}^{L} \frac{\alpha_l}{\beta c_l(\mathbf{X}^{\phi'})}\right) + \log(1 + \kappa(\theta))} \tag{19}$$

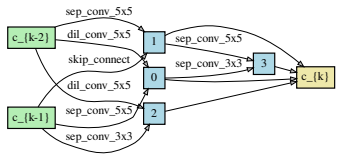
, where α_l is the total number of channels of the layer, β is the number of sampled channels, and $\mathbf{X}^{\phi'}$ is the concatenated feature map matrix using the sampled channels. This formulation restricts the dimension of the feature map matrix $\mathbf{X}^{\phi'}$ and eliminates the effect caused by the varying number of channels. We present the results of this optimisation procedure on the NATS-Bench-SSS benchmark in the Table 8. As observed, while Dextr_{opt} fixes the discrepancy for the NATS-Bench-SSS (Dong et al., 2021) benchmark, it fails to outperform the original formulation of Dextr in two out of three datasets.

A.3.2 MobileNet-v2

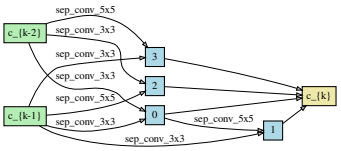
Our experiment on the MobileNet-v2 (Sandler et al., 2018) search space follows the standard evaluation protocol (Li et al., 2023; Lin et al., 2021; Lee & Ham, 2024) of searching for an architecture through evolutionary algorithm with FLOPs constraint of 450M. We use the same experimental settings as (Lee & Ham, 2024) with a population size of 1024 and a number of iterations as 1e5. Next, we train the selected architecture on ImageNet and report the floating point operations (FLOPs), Top-1 accuracy, and search cost in GPU Days in Table 9. We observe from the results that our method marginally improves over the previous best method AZ-NAS with a smaller searched model.

A.4 Implementation Details

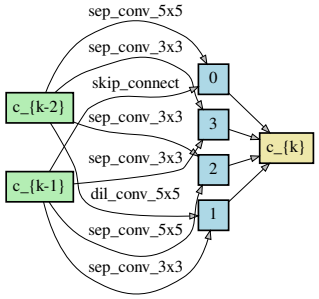
We now elaborate upon the procedure for the calculation of the Dextr value. First, we input a label-free data sample, i.e. an image from the CIFAR-10 dataset to a network from the respective benchmark and perform one forward pass with the image. In the forward pass, we calculate the sum of the inverse of the condition



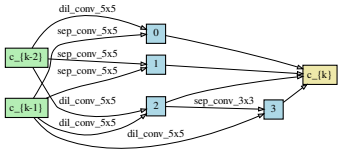
(a) MeCo (Jiang et al., 2023) (Normal cell)



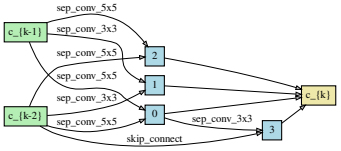
(b) ZiCo (Li et al., 2023) (Normal cell)



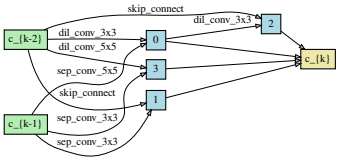
(c) Dextr (Normal cell) (ours)



(d) MeCo (Jiang et al., 2023) (Reduction cell)



(e) ZiCo (Li et al., 2023) (Reduction cell)



(f) Dextr (Reduction cell) (ours)

Figure 3: Found architectures from three zero cost proxies in the DARTS (Liu et al., 2019) search space for the ImageNet experiment using Zero-Cost-PT (Xiang et al., 2023).

number of the layer output for each layer, i.e. $(\sum_{l=1}^{L} 1/c_l(\mathbf{X}^{\phi}))$. Next, we obtain the extrinsic curvature $\kappa(\theta)$ by generating a random circular input and then calculating the velocity and acceleration vectors (Eq. 5). Finally, we calculate the Dextr value through Eq. 8.

A.5 Experimental settings

We run all the search procedures on a single NVIDIA RTX A6000 GPU with 48GB memory. For our correlation experiments on NAS-Bench-101 (Ying et al., 2019), NAS-Bench-301 (Zela et al., 2022), and TransNASBench-101 (Duan et al., 2021), we utilise the same experimental configuration as NAS-Bench-Suite-Zero (Krishnakumar et al., 2022), SWAPNAS (Peng et al., 2024). For our correlation experiments on NAS-Bench-201, we utilize the experimental setup as MeCo (Jiang et al., 2023). Moreover, the experimental configuration of the search on DARTS search space (Liu et al., 2019) using Zero-Cost-PT (Xiang et al., 2023) algorithm is detailed in Table 10. The training on ImageNet for DARTS search space follows the same settings and protocol as (Lukasik et al., 2022; Asthana et al., 2024; Chen et al., 2021c). Lastly, for our AutoFormer and MobileNet-v2 experiments, we utilize the same experimental framework as TF-TAS (Zhou et al., 2022) and AZ-NAS (Lee & Ham, 2024).

A.6 Visual Comparison

Figure 3 presents a visual comparison of the architectures generated by our proposed proxy, Dextr, alongside those produced by prior works, specifically MeCo (Jiang et al., 2023) and ZiCo (Li et al., 2023). The normal cell (used for feature extraction) generated by Dextr demonstrates a broad range of operations, including skip connections, separable convolutions, and dilated convolutions, while maintaining a densely connected structure. In contrast, the normal cell produced by MeCo exhibits simpler connections, which limits the network's expressivity. Similarly, although the normal cell generated by ZiCo features dense connections, it employs a less diverse set of operations compared to Dextr.

Table 10: Experimental settings for search in DARTS search space through Zero-Cost-PT algorithm.

Settings	Search settings
Batch Size	1
Cutout	False
Cutout Length	-
Learning Rate	0.025
Learning Rate Min	0.001
Momentum	0.9
Weight Decay	3e-4
Grad Clip	5
Init Channels	16
Layers	8
Drop Path Prob	-

Furthermore, the reduction cell (used for downsampling) generated by Dextr incorporates a more diverse set of operations. It effectively balances feature reuse through skip connections and flexible transformations utilizing dilated and separable convolutions. Thus, this design is particularly well-suited for complex tasks that require robust hierarchical representations.

A.7 Visualisation of correlation

We provide scatter plots between the Dextr score and the validation accuracy of the network across multiple correlation benchmarks, including NAS-Bench-101, NAS-Bench-201, NAS-Bench-301, and TransNAS-Bench-101-micro in Figure 4. All the plots reveal a strong positive correlation between the Dextr score and the performance of the network.

A.8 Limitations and Future Work

We now discuss some limitations of our work. Firstly, although our proxy does not require labelled data for computation, it still needs to perform slightly expensive calculations of the derivative of the output to compute the velocity $\mathbf{v}(\theta)$ and acceleration $\mathbf{a}(\theta)$ vectors, essential to calculate the expressivity of the network. Future works can focus on this issue by utilising a different characterisation of expressivity in the approach. Lastly, our theoretical analysis only applies to ReLU and GeLU networks. Extending the theoretical framework to other activation functions such as Sigmoid and Tanh can be an important future work direction. Lastly, Assumption 1 requires at least one absolute entry in $\mathbf{X}^{\phi}$ to be greater than 1. Although this is generally the case, some uncommon data normalisation tecnhniques can falsify this assumption.

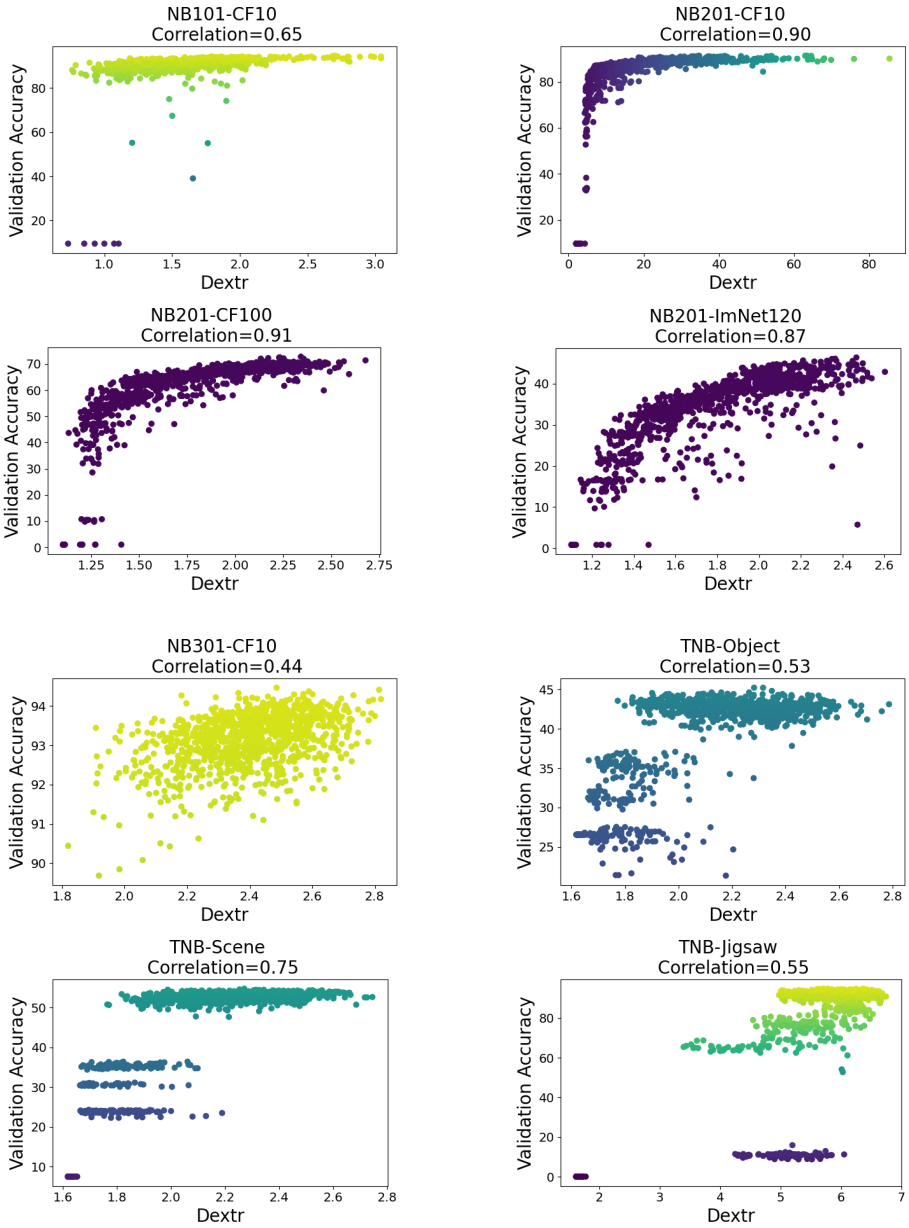


Figure 4: Scatter plots between Dextr value and validation accuracy for NAS-Bench-101 (Ying et al., 2019), NAS-Bench-201 (Dong & Yang, 2020), NAS-Bench-301 (Zela et al., 2022), and TransNAS-Bench-101-micro (Duan et al., 2021)