TRADITIONAL AND ACCELERATED GRADIENT DESCENT FOR NEURAL ARCHITECTURE SEARCH

NICOLÁS GARCÍA TRILLOS, FÉLIX MORALES, AND JAVIER MORALES

Abstract. In this paper, we introduce two algorithms for neural architecture search (NASGD and NASAGD) following the theoretical work by two of the authors [4], which aimed at introducing the conceptual basis for new notions of traditional and accelerated gradient descent algorithms for the optimization of a function on a semi-discrete space using ideas from optimal transport theory. Our methods, which use the network morphism framework introduced in [3] as a baseline, can analyze forty times as many architectures as the hill climbing methods [3, 11] while using the same computational resources and time and achieving comparable levels of accuracy. For example, using NASGD on CIFAR-10, our method designs and trains networks with an error rate of 4.06 in only 12 hours on a single GPU.

1. Introduction

Motivated by the success of neural networks in applications such as image recognition and language processing, in recent years practitioners and researchers have devoted great efforts in developing computational methodologies for the automatic design of neural architectures, in order to use deep learning methods in further applications. Roughly speaking, most approaches for neural architecture search (NAS) found in the literature build on ideas from reinforcement learning, evolutionary algorithms, and hill-climbing strategies– see section 1.1 for a brief review of the literature. All of these approaches attempt to address a central difficulty: the high computational burden of training multiple architecture models. Several developments in the design of algorithms, implementation and computational power, have resulted in methodologies that are able to produce neural networks that outperform the best networks designed by humans.

Despite all the recent exciting computational developments in NAS, we believe that is largely of interest to propose sound mathematical frameworks for the design of new algorithms. The goal is to use mathematical structures to guide the design of methodologies that can better explore the architecture space, achieving in this way higher accuracy rates in learning while reducing the computational burden of current methodologies.

In this paper we propose two new algorithms for NAS: neural architecture search gradient descent (NASGD) and neural architecture search accelerated gradient descent (NASAGD). These algorithms are based on the mathematical framework for semi-discrete optimization that two of the authors have introduced and motivated in their theoretical work [4], which attempted to answer the question:

How can one define a gradient for the optimization of an objective in the space $\mathbb{R}^d \times \mathcal{G}$ if $\mathcal{G}$ is a finite weighted graph?

Acknowledgements: N. García Trillos was supported by [nsf-dms 2005797]. The work of J. Morales was supported by NSF grants DMS16-13911, RNMS11-07444 (KI-Net) and ONR grant N00014-18-12465. The authors are grateful to the CSCAMM, to Prof. P.-E. Jabin and Prof. E. Tadmor for sharing with them the computational resources used to complete this work. Support for this research was provided by the Office of the Vice Chancellor for Research and Graduate Education at the University of Wisconsin-Madison with funding from the Wisconsin Alumni Research Foundation.
The answer provided in [4] is based on the idea of “lifting” the original semi-discrete optimization problem to one in the space of probability measures over $\mathbb{R}^d \times G$ where a Riemannian structure is available. Putting all technical details aside, at a high level neural architecture search can be seen as a semi-discrete optimization problem, where the discrete space can be interpreted as a space of architectures and where the continuous variable corresponds to the parameters associated to a given architecture. Both NASGD and NASAGD are inspired by the gradient flow structures introduced in [4].

The closest algorithm in the literature to the ones proposed here is the one presented in the work [3] which uses the concept of network morphism as a tool to introduce local graphs of architectures. It considers an iterative process where in a first step the weights of a collection of architectures are optimized for a fixed time, and in a second step the set of architectures are updated by applying morphisms to the best performing networks in the previous stage; these two steps are repeated until some stopping criterion is reached. While in our approaches we also use the concept of network morphism, the time spent in training a given set of networks is dynamically chosen as determined by an evolving particle system. In our numerical experiments we observe that our algorithms change architectures much earlier than the fixed amount of time proposed in [3], while achieving error rates of 4.06% on the CIFAR-10 data set trained over 12 hours with a single GPU for NASGD, and of 3.96% on the same training data set trained over 1 day with one GPU for NASAGD. Given the shorter time spent exploring architectures, both of our methodologies can be set to consider positive and negative architecture mutations, i.e. add/remove components to/from neural networks, as opposed to restricting to positive mutations as most approaches in the literature do. We believe that the improved exploration of the architecture space inherent to our algorithms can potentially be exploited further by combining it with reinforcement learning techniques. Namely, by mutating architectures more often, a controller may receive more data for training, ultimately producing a stronger controller which can the spend even less time training unfavorable architectures. This idea will be explored in more detail in the future.

Additionally, we would like to notice that while here we have restricted the use of the semi-discrete gradient dynamics introduced in [4] to the morphism framework from [3], we believe that our ideas have the potential to increase the quantity and speed at which architectures are explored in other NAS paradigms such as parameter sharing [8] and differential architecture search [1]. We will explore this direction in future work.

### 1.1. Review of neural architecture search frameworks and related works

There is an enormous literature on neural architecture search methodologies and some of its applications (see [13] for an overview on the subject). Roughly speaking, most methodologies found in the literature fall into the following families:

- **Reinforcement learning approaches.** The first group builds on ideas from reinforcement learning [15] and uses the concept of a controller/agent, who designs architectures (takes actions), trains them, and then receives rewards based on the performance of the trained networks. As in a typical reinforcement learning problem, the controller aims at maximizing a discounted future reward function. In this setting, the search for optimal policies corresponds to the design of architectures through gradient-based optimization of the future reward function using model-free methodologies such as REINFORCEMENT [12]. This reinforcement learning setting relies on two key components. Firstly, a neural network encoding/representation. This representation corresponds to deciding on a parameterization for the space of actions that the controller can take. Secondly, since the full training of a network is computationally expensive, different strategies need to be introduced to make the repeated evaluation of the reward function feasible. In the reinforcement learning setting from [15] these strategies are fundamental given that the computation of a single policy gradient step may involve the training of several neural architectures.
Evolutionary algorithms. The second major group of neural search methodologies is based on evolutionary algorithms [9, 10]. As in the reinforcement learning setting, evolutionary algorithms rely on suitable architecture encodings that facilitate the specification of rules for merging and mutation of different neural architectures. In the evolutionary setting, issues with competing conventions for the merging of two parent networks may arise. In order to address these issues, papers like [10] propose genetic encodings that depend on historical markings of mutations as they occur in an evolving population of architectures. The NEAT methodology from [10] offers a solution to the problem of competing conventions in diverse topologies. In evolutionary algorithms, the issue of evaluating an expensive objective is also present. Indeed, the evaluation of the fitness function used to determine what “individuals” should persist in time requires the full training of architecture models. Several strategies have been designed to address this issue. For example, a common technique is to evaluate the fitness function only at architecture candidates that are expected to return high fitness values. In turn, these candidates can be determined following strategies such as the covariance matrix evolution method from [5]. Originally this idea was applied in the context of neural networks for continuous hyperparameter optimization.

Some strategies used in the literature to lighten the computational burden of training multiple neural networks in NAS include:

- Parameter sharing approaches, see [8].
- Methods used on specific application domains, where architecture spaces are more concrete and thus specific strategies can be implemented, see [6].
- Techniques focused on transferring knowledge from simpler learning problems to more difficult ones, see [10].
- Strategies that use Bayesian model optimization, i.e. hyperparameter optimization techniques such as SMBO, see [6].
- Minimization of surrogate objectives, see [2, 14].

Another framework for NAS that is worth highlighting is the hill-climbing method introduced in [3]. There, the authors are motivated by similar considerations to ours and propose a climbing method to explore the discrete space of architecture models. Despite the similarities, our methodologies are markedly different in the way the architecture space is explored. First, we do not focus on the discrete space of architectures directly. Instead, our algorithms are inspired by particle methods that aim to mimic gradient flows on a space of probability measures where we gain access to differentiable structures as discussed in [4], allowing us to use a certain notion of gradient. Additionally, using the connections that our framework has with Riemannian geometry we are able to formulate analogs to accelerated gradient descent methods for the exploration of the space of architectures (this is the idea in NASAGD).

1.2. Outline. We organize the rest of the paper as follows. In section 2 we introduce our algorithms NASGD and NASAGD. To motivate them, we first discuss two particle dynamics used for the optimization of a function defined on a semi-discrete space \( \mathbb{R}^d \times G \) for \( G = (G, K) \) a finite weighted graph. In section 3 we compare the performance of NASGD and NASAGD against other NAS algorithms when working with the CIFAR-10 data set. In section 4 we provide more details on the implementation of our algorithms. In section 5 we provide some closing remarks and discuss future directions for research.

The appendix contains the two networks constructed by NASGD and NASAGD, and a slightly more detailed description of the particle dynamics that were used in our implementation.

2. Our algorithms

In this section, we introduce our algorithms NASGD and NASAGD. In order to describe them, for pedagogical purposes we first consider an idealized setting where we imagine that
NAS can be seen as a tensorized semi-discrete optimization problem of the form:

\[
\min_{(x,g) \in \mathbb{R}^d \times \mathcal{G}} V(x,g).
\]

In the above, it will be useful to think of the coordinate \( x \) as parameters and the coordinate \( g \) as an architecture. It will also be useful to think of \( \mathcal{G} = (\mathcal{G}, K) \) as a finite weighted graph of architectures, with \( K \) a matrix of positive weights characterizing “nearby architectures” (later on \( \mathcal{G} \) is defined in terms of network morphisms –see section 2.3), and \( V \) as a loss function (which for concreteness can be thought of as a cross-entropy loss function).

Working in this ideal setting, in the next two subsections we introduce particle systems that aim at solving (2.1). These particle systems are inspired by the gradient flow equations derived in [4]. In our actual implementation for CIFAR-10, we work with a modified version of the dynamics below (see section 4 and Appendix D). Such a version is more suitable in the context of deep learning, where the training data is on the order of \( 10^4 \) or more images.

### 2.1. First order algorithm.

The starting point of our discussion is equation (2.13) in [4] which reads:

\[
\begin{align*}
\frac{\partial f_t(x,g)}{\partial t} & = \Delta_x f_t(x,g) + \text{div}_x(f_t(x,g) \nabla_x V(x,g)) \\
& + \sum_{g' \in \mathcal{G}} \left[ \log f_t(x,g) + V(x,g) - (\log f_t(x,g') + V(x,g')) \right] K(g,g') \theta_{x,g,g'}(f_t(x,g), f_t(x,g')),
\end{align*}
\]

and describes the evolution in time of a joint distribution on \((x,g)\) (here denoted with \(f_t(x,g)\)), that can be interpreted as the gradient descent dynamics (in continuous time) of the relative entropy energy

\[
\mathcal{E}(f) := \sum_{g \in \mathcal{G}} \int_{\mathbb{R}^d} \log f(x,g) f(x,g) + \sum_{g} \int_{\mathbb{R}^d} V(x,g) f(x,g),
\]

with respect to a Riemannian structure discussed in detail in [4]. In simple words, we can imagine that (2.1) is a gradient descent algorithm for the minimization of \( \mathcal{E} \) – see section 2.3 in [4]. In the energy \( \mathcal{E} \) the entropic term (the first one) encourages exploration of the space \( \mathbb{R}^d \times \mathcal{G} \), while the potential energy (the second term) favors distributions that concentrate on regions with low values of \( V \).

In order to restrict “wandering” to the \( g \) coordinate only, one can consider modifying the energy \( \mathcal{E} \) slightly by replacing the entropic term that acts on both variables \((x,g)\) with the entropy of just the marginal on the \( g \) variable, i.e. consider the energy

\[
\tilde{\mathcal{E}}(f) := \sum_{g \in \mathcal{G}} \log f(g) f(g) + \sum_{g} \int_{\mathbb{R}^d} V(x,g) f(x,g),
\]

where we interpret \( f(g) \) as the marginal on the \( g \) coordinate of the joint distribution \( f(x,g) \). The steepest descent equations for the minimization of \( \tilde{\mathcal{E}} \) using the Riemannian structure discussed in section 2.3 in [4] take the form:

\[
\begin{align*}
\frac{\partial f_t(x,g)}{\partial t} & = \text{div}_x(f_t(x,g) \nabla_x V(x,g)) \\
& + \sum_{g' \in \mathcal{G}} \left[ \log f_t(g) + V(x,g) - (\log f_t(g') + V(x,g')) \right] K(g,g') \theta_{x,g,g'}(f_t(x,g), f_t(x,g')).
\end{align*}
\]

For practical purposes, this equation is a better starting point to motivate algorithms for the optimization of the function \( V \). Indeed, by only allowing “wandering” in the \( g \) coordinate, we can take advantage of the many gradient descent strategies that have been introduced in the literature for the training of neural networks (i.e. optimizing over \( x \) without having to add noise), while still encouraging exploration of the architecture space.

How can one make use of the above dynamics to motivate algorithms for the optimization of the function \( V \)? One possibility is to consider a collection of moving particles on \( \mathbb{R}^d \times \mathcal{G} \) whose evolving empirical distribution aims at mimicking the evolution described in (2.5). Let us then suppose that \( N \) particles are allowed to move in \( \mathbb{R}^d \times \mathcal{G} \) and that initially they have locations
\((x_i, g_i) = 1, \ldots, N\) where we assume that if \(g_i = g_j\) then \(x_i = x_j\). The locations are then updated by repeatedly applying the following steps:

- **Step 1: Updating parameters (Training):** For each particle \(i\) with position \((x_i, g_i)\) we update its parameters by setting:
  \[ x_i^T = x_i - \tau \nabla_x V(x_i, g_i). \]

- **Step 2: Moving in the architecture space (Mutation):** First, for each of the particles \(i\) with position \((x_i, g_i)\) we decide to change its \(g\) coordinate with probability:
  \[ \tau \sum_j (\log f(g_j) + V(x_j, g_j)) - (\log f(g_i) + V(x_i, g_i)) - K(g_i, g_j), \]
  or 1 if the above number is greater than 1. If we decide to move particle \(i\), we move it to the position of particle \(j\), i.e. \((x_j, g_j)\), with probability:
  \[ f \left( \frac{\left[ \log f(g_j) + V(x_j, g_j) - (\log f(g_i) + V(x_i, g_i)) \right] - K(g_i, g_j)}{\sum_i \left[ \log f(g_i) + V(x_i, g_i) - (\log f(g_i) + V(x_i, g_i)) \right] - K(g_i, g_j)} \right). \]

In the above \(f(g)\) denotes the ratio of particles that are located at \(g\). Additionally, \(a^- = \max\{0, -a\}\) denotes the negative part of the quantity \(a\).

**Remark 2.1.** Notice that given the assumption on the initial locations of the particles, throughout all the iterations of Step 1 and Step 2 we make sure that if \(g_i = g_j\) then \(x_i = x_j\).

**Remark 2.2.** It is worth remarking that the particle dynamics described in Step 1 and Step 2 although inspired by [25], are perhaps more closely related to the gradient flow of the energy \(\tilde{E}\) with respect to a Finslerian structure analogous to the Riemannian structure considered in [4]. A more detailed discussion on this is out of the scope of this paper.

**Remark 2.3.** By modifying the energy \(\tilde{E}(f)\) replacing the entropic term with an energy of the form \(\frac{1}{\beta+1} \sum_g (f(g))^\beta+1\) for some parameter \(\beta > 0\), one can motivate a new particle system where in Step 2 every appearance of \(\log f\) is replaced with \(f^\beta\). The effect of this change is that the resulting particle system moves at a slower rate than the version of the particle system as described in Step 2.

### 2.2. Second order algorithm.

Our second order algorithm is inspired by the system of equations (2.17) in [4] which reads

\[
\begin{align*}
\partial_t f_i(x, g) + \text{div}_x (f_i(x, g) \nabla_x \varphi_t) + \sum_{g'} (\varphi_t(x, g') - \varphi_t(x, g)) K(g, g') \theta_{x,g,g'}(f_i(x, g), f_i(x, g)) = 0 \\
\partial_t \varphi_t + \frac{1}{2} |\nabla_x \varphi_t|^2 + \sum_{g'} (\varphi_t(x, g) - \varphi_t(x, g'))^2 K(g, g') \partial_t \theta_{x,g,g'}(f_i(x, g), f_i(x, g')) = -[\gamma \varphi_t(x, g) + \log f_i(x, g) + V(x, g)],
\end{align*}
\]

and describes what can be considered as a second order algorithm for the optimization of the relative entropy \(E\) – see sections 2.4 and 3.3. in [4] for a detailed discussion. Here, \(f_i(x, g)\) is again a joint distribution on \((x, g)\), and the function \(\varphi_t\) is a real valued function over \(\mathbb{R}^d \times \mathcal{G}\) that can be interpreted as the momentum variable. \(\gamma \geq 0\) is a friction parameter.

As in the first order case, we may consider the optimization of the modified energy \(\tilde{E}\) instead of \(E\) now following second order dynamics. The resulting system of equations motivates the following particle system, where now we think that the position of a particle is characterized by the tuple \((x_i, g_i, v_i)\) where \(x_i, v_i \in \mathbb{R}^d\), \(g_i \in \mathcal{G}\), and in addition we have a potential function \(\varphi : \mathcal{G} \to \mathbb{R}\) that also gets updated. Initially, we assume that if \(g_i = g_j\) then \(x_i = x_j\) and \(v_i = v_j\), and that \(\varphi\) is identically equal to zero.
We summarize the second order gradient flow dynamics as the iterative application of three steps:

- **Step 1: Updating parameters (Training):** For each particle $i$ located at $(x_i, g_i, v_i)$ we update its parameters $x_i, v_i$ by setting

\[
x_i^t = x_i + \tau v_i,
\]

\[
v_i^t = v_i - \tau (\gamma v_i + \nabla_x V(x_i, g_i)).
\]

- **Step 2: Moving in the architecture space (Mutation):** First, for each of the particles $i$ with position $(x_i, g_i, v_i)$ we decide to move it with probability

\[
\tau \sum_j (\varphi(g_i) - \varphi(g_j))^-K(g_i, g_j),
\]

or 1 if the above quantity is greater than 1. Then, if we decided to move the particle $i$ we move it to location of particle $j$, $(x_j, g_j, v_j)$ with probability:

\[
(\varphi(g_i) - \varphi(g_j))^-K(g_i, g_j) \times \left(\sum_i (\varphi(g_i) - \varphi(g_i))^-K(g_i, g_i)\right)^{-1}.
\]

- **Step 3: Updating momentum on the $g$ coordinate:** We update $\varphi$ according to:

\[
\varphi^\tau(g_i) = \varphi(g_i) - \frac{\tau}{2} |v_i|^2 - \tau \left(\sum_j (\varphi(g_i) - \varphi(g_j))^-|^2 K(g_i, g_j)\right)
- \tau (\gamma \varphi(g_i) + \log f(g_i) + V(x_i, g_i)),
\]

for every particle $i$. Here, $f(g)$ represents the ratio of particles located at $g$.

**Remark 2.4.** Notice that given the assumption on the initial locations of the particles, throughout all the iterations of Step 1 and Step 2 and Step 3 we make sure that if $g_i = g_j$ then $x_i = x_j$ and $v_i = v_j$.

### 2.3. NASGD and NASAGD.

We are now ready to describe our algorithms NASGD and NASAGD:

**Algorithm 1 NASGD**

1. Load an initial architecture $g_0$ with initial parameters $x_0$ and set $r = 0$.
2. Construct a graph $G_r$ around $g_r$ using the notion of network morphism introduced in [3]. More precisely, we produce $n_{neigh}$ new architectures with associated parameters, each new architecture is constructed by modifying $g_r$ using a single network morphism from [3]. Then define $G_r$ as the set consisting of the loaded $n_{neigh}$ architectures and the architecture $g_r$. Set the graph weights $K(g, g')$ (for example, setting all weights to one).
3. Put $N$ particles on $(x_r, g_r)$ and put 1 “ghost” particle on each of the remaining architectures in $G_r$. The architectures for these ghost particles are never updated (to make sure we always have at least one particle in each of the architectures in $G_r$), but certainly their parameters will.

Then, run the dynamics discussed in section 2.1 on the graph $G_r$ (or the modified dynamics see, Remark 2.3 and Appendix D) until the node in $G_r \setminus \{g_r\}$ with the most particles $g_r^{max}$ has twice as many particles as $g_r$.

Set $r = r + 1$. Set $g_r = g_r^{max}$ and $x_r = x_r^{max}$, where $x_r^{max}$ are the parameters of architecture $g_r^{max}$ at the moment of stopping the particle dynamics.

4. If size of $g_r$ exceeds a prespecified threshold (in terms of number of convolutional layers for example) go to 5. If not go back to 2.
5. Train $g_r$ until convergence.
Algorithm 2 NASAGD

1. Load an initial architecture $g_0$ with initial parameters $x_0$ and $v_0$. Set $\varphi_0 \equiv 0$. Set $r = 0$.
2. Construct a graph $G_r$ around $g_r$ using the notion of network morphism introduced in [3]. More precisely, we produce $n_{\text{neigh}}$ new architectures with associated parameters, each new architecture is constructed by modifying $g_r$ using a single network morphism from [3]. Then define $G_r$ as the set consisting of the loaded $n_{\text{neigh}}$ architectures and the architecture $g_r$. Set the graph weights $K(g,g')$ (for example, setting all weights to one).
3. For NASGD: Locate $N$ particles on $(x_r, g_r, v_r)$, and put 1 “ghost” particle on each of the remaining architectures in $G_r$. The architectures for these ghost particles are never updated (to make sure we always have at least one particle in each of the architectures in $G_r$), but certainly their parameters will.

   Initialize the potential $\varphi_r$ to 0. Then run the dynamics discussed in section 2.6 (or the modified dynamics see, Remark 2.3 and Appendix D) until the node in $G_r \setminus \{g_r\}$ with the most particles $g_{\text{max}}$ has twice as many particles as $g_r$.

   Set $r = r + 1$. Set $g_r = g_{\text{max}}$, $x_r = x_{\text{max}}$, $v_r = v_{\text{max}}$ where $x_{\text{max}}, v_{\text{max}}$ are the parameters of architecture $g_{\text{max}}$ at the moment of stopping the particle dynamics.
4. If size of $g_r$ exceeds a prespecified threshold (in terms of number of convolutional layers for example) go to 5. If not go back to 2.
5. Train $g_r$ until convergence.

3. Experiments

In this section, we present our numerical results. Before displaying them, we compare in more detail our algorithms with the ones proposed in [3] and [11]. We have decided to focus on these methodologies since, in the literature, they are the closest to our approach. We begin by summarizing their framework and explaining how we apply our gradient flow dynamics to it.

- **Hill climbing and graph search framework**: The algorithm proposed in [3] starts with a small pre-trained network. The authors then suggest an application of a fixed number $n_{\text{NM}}$ of random network morphisms to this base network to produce $n_{\text{neigh}}$ children networks. They train the children networks during $\text{epochs}_{\text{neigh}}$ epochs using SGD and the cosine annealing strategy introduced in [7]. The learning rate is interpolated from $\lambda_{\text{start}}$ to $\lambda_{\text{final}}$ during the $\text{epochs}_{\text{neigh}}$ epochs. Their algorithm iterates this process, restarting it $n_{\text{steps}}$ times. At the beginning of each cycle, it applies the same number of morphisms to the best performing architecture in the previous cycle to produce new $n_{\text{neigh}}$ children architectures. After the $n_{\text{steps}}$ cycles, the best network is trained until convergence using the same range for the cosine aliasing. The work [11] builds upon the framework introduced in [3] by including linear morphisms and gradient weighting techniques that prevent old layers from overfitting.

Next, we describe how we use our first and second-order architecture search algorithms NASGD and NASAGD to perform our numerical experiments.

- **Our framework for NASGD and NASAGD**: In a similar way to [3] and [11], we pre-train an initial network $g_0$ with the structure Conv-MaxPool-Conv-MaxPool-Softmax for 20 epochs using cosine aliasing that interpolates between 0.5 and $10^{-7}$. We use $g_0$ with parameters $x_0$ as the initial data for our gradient flow dynamics introduced in section 2.1 for the first-order algorithm NASGD and section 2.6 for the second-order algorithm NASAGD. During the NASGD and NASAGD algorithms, we use cosine aliasing interpolating the learning rate from $\lambda_{\text{start}}$ to $\lambda_{\text{final}}$ with a restart period of $\text{epochs}_{\text{neigh}}$. In contrast to the NASH approach from [3], since we initialize new architectures, we do not reset the time step along with the interpolation for the $\text{epochs}_{\text{neigh}}$ epochs. Our
particle system *dynamically* determines the number of initialization. We continue this overall dynamics, resetting the learning rate from $\lambda_{\text{start}}$ to $\lambda_{\text{final}}$ every $\text{epochs}_{\text{neigh}}$ at most $n_{\text{steps}}$ times. We perform several experiments letting the first and second-order gradient flow dynamics run for different lengths of time. Finally, we train the found architectures until convergence.

**Remark 3.1.** Here, by Conv, and throughout the rest of the paper we mean:

$$\text{Conv} = \text{Conv} + \text{batchnorm} + \text{Relu},$$

### 3.1. Models found by our NASGD and NASAGD algorithms.

In our numerical experiments, we find two models NASGD1 and NASAGD1 (see Appendix 5 and 11 respectively). We found the model NASGD1 running the first-order gradient flow dynamics with $n_{\text{steps}} = 0.89$. On the other hand, we obtain the model NASAGD1, by running the second-order gradient flow dynamics with $n_{\text{steps}} = 2.54$. In the table below, we display the rest of the parameters used to find these models. We also present the corresponding parameters used to find the NASH2 model obtained from [3] and the NASGraph model from [11]:

| Variable          | NASH2 | NASGraph | NASGD1 | NASAGD1 |
|-------------------|-------|----------|--------|---------|
| $n_{\text{steps}}$ | 8     | 10       | 0.89   | 2.54    |
| $n_{\text{NM}}$   | 5     | 5        | dynamic| dynamic |
| $n_{\text{neigh}}$| 8     | 8        | 8      | 8       |
| $\text{epoch}_{\text{neigh}}$ | 17    | 16       | 18     | 18      |
| $\lambda_{\text{start}}$ | 0.05  | 0.1      | 0.05   | 0.05    |
| $\lambda_{\text{final}}$ | 0     | 0        | $10^{-7}$ | $10^{-7}$ |
| Gradient Stopping | No    | Yes      | No     | No      |

For the reader’s convenience, we summarize below the meaning of each of the variables in the above table:

- $n_{\text{steps}}$ denotes the number of restart cycles for the cosine aliasing.
- $n_{\text{NM}}$ is the number of morphism operations applied on a given restart cycle.
- $n_{\text{neigh}}$ is the number of children architectures generated every time the current best model changes.
- $\text{epoch}_{\text{neigh}}$ is the number of epochs that go by before the cosine aliasing is restarted.
- $\lambda_{\text{final}}$ and $\lambda_{\text{start}}$ are the parameters required for SGDR.

### 3.2. Numerical Results.

We performed two experiments to produce NASGD1 and NASAGD1, which respectively used the first and second order algorithms to learn from the CIFAR-10 data set. We compare the performance of our methodologies against NASH2 and NasGraph.

| Numerical Experiment | CIFAR 10 model | resources | # params ×10⁶ | error |
|----------------------|----------------|-----------|---------------|-------|
| NASH2                | 1GPU, 1 day    | 19.7      | 5.2           |
| NASGraph             | 1GPU, 20 h     | ?         | 4.96          |
| NASGD1               | 1GPU, 12h      | 25.4      | 4.06          |
| NASAGD1              | 1GPU, 1 day    | 22.9      | 3.96          |

As can be observed from the above table, our algorithms are competitive with state of the art methods. It is worth highlighting that our algorithms can explore more considerably architectures (about a 40 times more) with the same computational resources. We also notice that in contrast to the framework [3], we consider positive as well as negative mutations, i.e., mutations that can increase or decrease the number of filters, layers, skip, and dimension of convolutional kernels.
4. FINE-TUNING OF THE FIRST AND SECOND-ORDER GRADIENT FLOW DYNAMICS

In this section, we explain the main points that need to be modified from the gradient flow dynamics from sections 2.1 and 2.2 in order to make them better suited for the NAS problem. In particular, these adaptations are implemented in order to make our algorithms viable for learning from the CIFAR-10 data set where we deal with $10^4$ or more labeled images, and where overfitting to the data might certainly be an issue. For the reader’s convenience, we have stated the equations for the final version of our dynamics in Appendix D. We fine-tune these dynamics by addressing the following points:

4.1. Stochastic gradient descent and decoupling of the loss function: The first adaptation we make is to consider a stochastic gradient descent version of the dynamics proposed in sections 2.1 and 2.2. To perform stochastic gradient descent we first need a sequence of mini-batches $\{X_k\}_k$ (of the same size) that are randomly chosen from our labeled training data set. We denote the batch size with $S_X$. In our experiments, we set $S_X = 64$. In each iteration of our dynamics, for the training step we will use one of these mini-batches $X_k$ (we technically use different mini-batches for each architecture, but for notational simplicity, let us pretend it is the same for all architectures in each iteration) in order to define the loss function to be optimized (more details below). We will use a different sequence of mini-batches $\{Y_k\}_k$, which we will build from a set, disjoint from the one used to build the $\{X_k\}_k$. These mini-batches are used in the validation of the network performance. In our implementation, we set the size of these validation mini-batches to be $S_Y = 32$. Keep in mind that the data in the $Y_k$ are never used to update network parameters.

More precisely we do the following:

(a) *Adaptation of the training step:* During the training step of our algorithm, when we are updating the parameters of an architecture $g$ with parameters $x$, we denote the value of the forward feed of $g$ evaluated at the mini-batch $X_k$ with $V_k(x,g)$. Then, at the $k$-th step we update the parameters of the network $(x,g)$ with the gradient $\nabla x V_k(x,g)$.

(b) *Adaptation of the mutation step:* For this step we will use the validation mini-batches $\{Y_k\}_k$. That is, given an architecture $g$ with parameters $x$ that is loaded on the $k$-th iteration, we denote the value of the forward feed of $g$ evaluated at the mini-batch $Y_k$ by $\tilde{V}_k(x,g)$. In appendix D we rewrite our mutation steps in terms of $\tilde{V}$ valuations. We notice that in the hill-climbing framework [3], the authors use the accuracy on the validation set to determine the best model. Similarly, we define $\tilde{V}$ using mini-batches sampled from a validation set (we reiterate that we do not use these mini-batches in the training step). In this way, the mutation step assigns particles to those architectures that are better at generalizing their training to sets that are disjoint from the training set. Empirically, we found that this increases accuracy and prevents overfitting.

4.2. Warm restarts and final adaptation of the dynamics: As discussed in [3], the training step discussed in section 2.1 is generally not fast enough to produce significant variations between architectures in a reasonable time. Hence, for the experiment NASGD1, we have used the technique in [7] and perform the training with momentum and cosine aliasing. In Appendix D we denote the size of the time step determined by the cosine aliasing in the $k$-th iteration by $\tau_k$.

For the mutation steps in both the first and second order models we followed Remark 2.3 in order to slow down the propagation of particles. We found that this choice produced better results than the original particle system described in sections 2.1 and 2.2 – see Appendix D for a more detailed formulation of our particle system. Also, for the mutation step of the second-order model, we do not use the term $\frac{1}{2} |v_1|^2$ since it is quite expensive to compute, and empirically was observed to not affect our final results significantly.
4.3. **Constraining the graph of architectures:** We adopt a similar strategy to [11] to dynamically modify the size of the last layer of our network before the fully connected part. Additionally, we impose global constraints on loaded architectures such as a maximum number of pool layers and filters. We also constrain the number of incoming connections that a given layer may receive.

**Remark 4.1.** In contrast to [3], we apply a single morphism at the same time. We can afford this because our particle dynamics sample more architectures overall. On the other hand, this choice was somewhat arbitrary, and it could be productive to randomize the number of morphisms applied in order to produce new competing architectures at the beginning of each cycle. Additionally, we have considered morphisms that may reduce the size of our network. Architectures produced by negative morphisms are occasionally preferred by the particle dynamics.

5. **Conclusions and discussion**

In this work, we have proposed novel first and second order gradient descent algorithms for neural architecture search (NASGD and NASAGD). The theoretical gradient flow structures in the space of probability measures over a semi-discrete space introduced in [4] serve as the primary motivation for our algorithms. Our numerical experiments show the practical viability of our methodologies: we achieve competitive results, while analyzing a considerably larger amount of architectures using the same computational resources as state of the art methods.

The methodologies introduced in this paper are part of a first step in a broader program where we envision the use of well defined mathematical structures to motivate new NAS algorithms. Although here we have achieved competitive results, we believe that there are still several possible directions for improvement that are worth exploring in the future.

We believe that a source of improvement for the algorithms that have been proposed in this paper may come from a more careful analysis of some of the hyperparameters chosen to tune them. For example, in our methodologies we have considered morphisms that can increase and decrease the size of a network, but perhaps unsurprisingly we have empirically observed that our algorithms prefer larger architectures over smaller ones. Selecting a single morphism was a somewhat arbitrary choice that may not lead us in the direction of a global optimum, as in principle it will be difficult to return to basic architectures once complex ones are being analyzed. It is then of interest to have a better understanding of the number of morphisms that should be considered at each step of our algorithms, and in general to better understand the degree of freedom that comes when building the local graphs $G_r$. Mutation and training coefficients are other parameters that need to be better understood.

A more careful analysis and tuning of hyperparameters for NASAGD are of particular interest so as to help clarify its relative strengths with respect to NASGD. We do not believe that our numerical experiments have been conclusive about the advantages/disadvantages of NASAGD.

Given that our methods have the added advantage that they can analyze a much larger number of architectures with the same resources used by the approaches in [3] and [11], we believe that our methods have the potential to develop a strong synergy with reinforcement learning approaches. In reinforcement learning methods, a controller learns from data collected as architectures are explored. As data gets collected faster, a trained controller may in principle better predict morphism chains, improving in this way the construction of local graphs.

A final research direction that stems from our work is motivated by the task of neural network distillation (or pruning). Indeed, by considering negative morphisms only, we may actually use the same particle dynamics used to explore local graphs in order to prune complex neural networks in search of simpler networks with good accuracy rates. This direction will be explored in future work.
References

[1] DARTS: differentiable architecture search. CoRR, abs/1806.09055, 2018.
[2] J. S. Bergstra, R. Bardenet, Y. Bengio, and B. Kégl. Algorithms for hyper-parameter optimization. In J. Shawe-Taylor, R. S. Zemel, P. L. Bartlett, F. Pereira, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 24, pages 2546–2554. Curran Associates, Inc., 2011.
[3] T. Elsken, J.-H. Metzen, and F. Hutter. Simple and efficient architecture search for convolutional neural networks, 2017.
[4] N. Garcia-Trillos and J. Morales. Semi-discrete optimization through semi-discrete optimal transport: a framework for neural architecture search. https://arxiv.org/abs/2006.15221, 2020.
[5] N. Hansen. The cma evolution strategy: A tutorial. ArXiv, abs/1604.00772, 2008.
[6] C. Liu, B. Zoph, M. Neumann, J. Shlens, W. Hua, L.-J. Li, L. Fei-Fei, A. Yuille, J. Huang, and K. Murphy. Progressive neural architecture search. In V. Ferrari, M. Hebert, C. Sminchisescu, and Y. Weiss, editors, Computer Vision – ECCV 2018, pages 19–35, Cham, 2018. Springer International Publishing.
[7] I. Loshchilov and F. Hutter. Sgdr: Stochastic gradient descent with warm restarts. In ICLR, 2017.
[8] H. Pham, M. Guan, B. Zoph, Q. Le, and J. Dean. Efficient neural architecture search via parameters sharing. In J. Dy and A. Krause, editors, Proceedings of the 35th International Conference on Machine Learning, volume 80 of Proceedings of Machine Learning Research, pages 4095–4104, Stockholmsmssan, Stockholm Sweden, 10–15 Jul 2018. PMLR.
[9] E. Real, A. Aggarwal, Y. Huang, and Q. V. Le. Regularized evolution for image classifier architecture search. In AAAI, 2018.
[10] K. O. Stanley and R. Miikkulainen. Evolving neural networks through augmenting topologies. Evolutionary Computation, 10(2):99–127, 2002.
[11] M. Verma, P. Sinha, K. Goyal, A. Verma, and S. Susan. A novel framework for neural architecture search in the hill climbing domain. In 2019 IEEE Second International Conference on Artificial Intelligence and Knowledge Engineering (AIKE), pages 1–8, 2019.
[12] R. Williams. Simple statistical gradient-following algorithms for connectionist reinforcement learning. Mach Learn 8, 8:229256, 1992.
[13] T. Yu and H. Zhu. Hyper-parameter optimization: A review of algorithms and applications, 2020.
[14] T. Yu and H. Zhu. Hyper-parameter optimization: A review of algorithms and applications. ArXiv, abs/2003.05689, 2020.
[15] B. Zoph and Q. V. Le. Neural architecture search with reinforcement learning, 2016.
[16] B. Zoph, V. Vasudevan, J. Shlens, and Q. V. Le. Learning transferable architectures for scalable image recognition, 2017.
Appendix A. Architecture found by the NASGD algorithm

conv0 → conv1 → (pool0) → conv2 → conv3 → (pool1) → conv4 → (pool2) → (conv5) → (conv6) → (conv7) → (conv8) → (conv9) → (conv10) → (conv11) → (conv12) → (conv13) → (conv14) → (conv15) → (conv16) → (conv17) → (conv18)
Appendix B. Architecture found by the NASAGD algorithm
Appendix C. Learning curve for the NASGD1 and NASAGD1 experiments

![Graph showing learning curve for NASGD1 and NASAGD1 experiments]

**Figure 1.** On this plot, we display the accuracy of the current best-performing epochs during \( n_{\text{steps}} = 0.89 \) cycles of the architecture search part of the algorithm. NASGD finds our model during this time and then trains it until it reaches the error rate of 4.06.

Appendix D. Implemented particle methods

In this section, for the convenience of the reader, we write the final equations for the adapted dynamics from sections 2.1 and 2.2 after all the points discussed in section 4 are considered.

D.1. First order algorithm (NASGD). We summarize the first order gradient flow dynamics as the iterative application of the following two steps:

- **Step 1: Updating the parameters (Training):** For each of the previously initialized networks \((x_i, g_i, v_i)\) we compute \(V_k(x_i, g_i)\), and \(\nabla_x V_k(\cdot, g_i)\), and update its parameters by setting

\[
x_{i}^{\tau_k} = x_{i} + \tau_k v_{i},
\]

\[
v_{i}^{\tau_k} = v_{i} - \tau_k (v_{i} + \nabla_x V_k(x_i, g_i)).
\]

Here, and henceforth, we use \(\tau_k\) to denote the length of the time step determined by the global cosine aliasing interpolation. Similarly, \(V_k(g_i, x)\) denotes the valuation function of the current mini-batch for the stochastic gradient descent. Note that as described in section 4, we use second order dynamics for the training even though technically speaking we are stating our first order approach.
- **Step 2: Moving the particles (Mutation):** First, for each particle at each initialized network \((x, g)\), we select to move it, with probability

\[ \kappa \tau_k \sum_{g'} \left[ (f^\beta(g') + \tilde{V}_k(x', g')) - (f^\beta(g) + \tilde{V}_k(x, g)) \right]^+ K(g, g'), \]

or 1 if the above quantity is greater than 1. Here, \(\kappa > 0\) denotes the mutation coefficient. As discussed in section 4, \(\tilde{V}_k\) is used to denote the running average of the valuation of the lost function in the respective mini-batches of a given architecture.

Then, if we decide to move a particle in \((x, g)\) we move it to \((x', g')\) with probability,

\[ \left( \frac{\left[ f^\beta(g') + \tilde{V}_k(x', g') - (f^\beta(g) + \tilde{V}_k(x, g)) \right]^+ K(g, g')}{\left( \sum_{g''} \left[ f^\beta(g'') + \tilde{V}_k(x'', g'') - [f^\beta(g) + \tilde{V}_k(x, g)] \right]^+ K(g, g'') \right)} \right). \]

D.2. **Second order algorithm (NASAGD):** We summarize the second order gradient flow dynamics as the iterative application of the following three steps:

- **Step 1: Updating the parameters (Training):** For each of the previously initialized networks \((x_i, g_i, v_i)\) we compute \(V_k(x_i, g_i)\), compute its gradient \(\nabla_x V_k(\cdot, g_i)\), and update its parameters by setting

\[ x_{i\tau_k} = x_i + \tau_k v_i, \]
\[ v_{i\tau_k} = v_i - \tau_k (v_i + \nabla_x V_k(x_i, g_i)). \]

- **Step 2: Moving the particles (Mutation):** First, for each particle at \((x, g, v)\), we move it with probability

\[ \kappa \tau_k \sum_{g'} (\varphi(g) - \varphi(g'))^{-1} K(g, g'), \]

or 1 if the above quantity is greater than 1. Then, if we decided to move the particle, we move it to \((x', g', v')\) with probability:

\[ (\varphi(g) - \varphi(g'))^{-1} K(g, g') \times \left( \sum_{g''} (\varphi(g) - \varphi(g''))^{-1} K(g, g'') \right)^{-1}. \]

- **Step 3: Updating the velocity field (applying external force):** To do this, we set

\[ \varphi^\tau_k(g) = \varphi(g) - \tau_k \left( \sum_{K(g', g)} \left( [\varphi(g) - \varphi(g')]^{-1} K(g, g') \right)^2 \right) \]
\[ - \tau_k (f^\beta(g) + \tilde{V}_k(x, g)), \]

for each previously initialized architecture \(g\).

During our implementation, we found it useful to restart \(\varphi\) and set it equal to 0 every time that the quantity

\[ \sum_{g, g'} (\varphi(g) - \varphi(g'))^{-1} \cdot (\tilde{V}_k(x, g) - \tilde{V}_k(x', g'))^{-1} K(g, g') f(g), \]

becomes positive. Heuristically, this quantity measures the rate of change of the average loss function for all the particles as they evolve in time.
Nicolás García Trillos, Department of Statistics, University of Wisconsin-Madison. 1300 University Avenue, Madison, WI, USA 53706, E-mail address: garciatrillo@wisc.edu

Félix Morales, Departmento de Ingeniería Informática, Universidad Católica Andrés Bello, Caracas 1000, Capital District, Venezuela, E-mail address: famorales.14@est.ucab.edu.ve

Javier Morales, Center for Scientific Computation and Mathematical Modeling (CSCAMM), University of Maryland, College Park MD 20742, E-mail address: javierm1@cscamm.umd.edu