

# Multi-objective Differentiable Neural Architecture Search

Rhea S. Sukthanker<sup>1\*</sup>

Arber Zela<sup>1\*</sup>

Benedikt Staffler<sup>2</sup>

Samuel Dooley<sup>3</sup>

Josif Grabocka<sup>4</sup>

Frank Hutter<sup>1</sup>

<sup>1</sup> University of Freiburg

<sup>2</sup> Bosch Center for Artificial Intelligence

<sup>3</sup> Abacus AI

<sup>4</sup> University of Nürnberg

February 24, 2025



GEFÖRDERT VOM



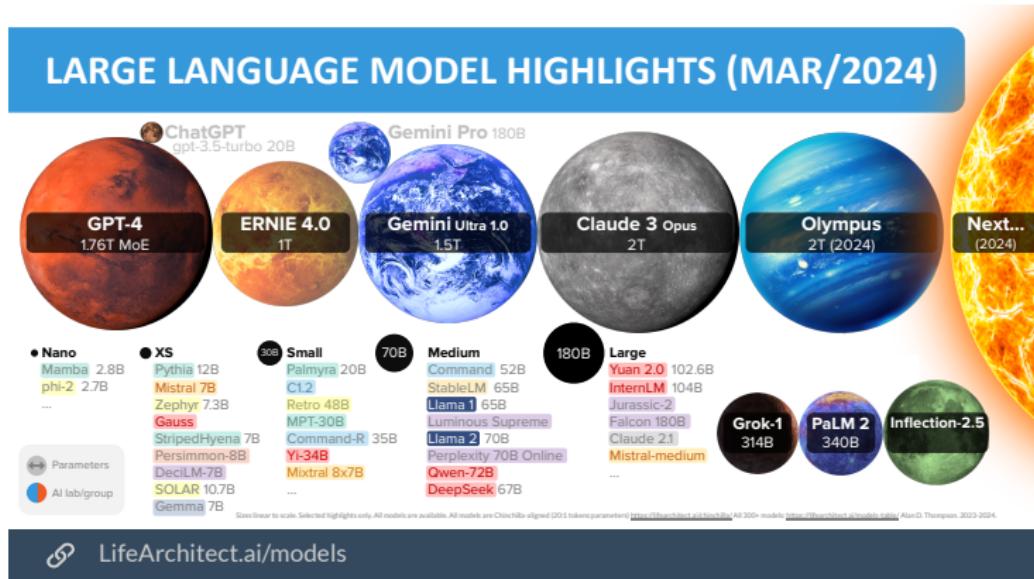
# NAS in a world of ever growing models

- In an age of **large models**, finding architectures which are *performant*, *efficient* and with *fast* inference times is pivotal.



# NAS in a world of ever growing models

- In an age of **large models**, finding architectures which are *performant*, *efficient* and with *fast* inference times is pivotal.



# NAS in a world of ever growing models

- In an age of **large models**, finding architectures which are *performant*, *efficient* and with *fast* inference times is pivotal.
- Multi-objective problem with (potentially) **conflicting objectives**.
  - Optimizing all objectives simultaneously is infeasible.
  - Finding the **right trade-off** remains challenging.



# NAS in a world of ever growing models

- In an age of **large models**, finding architectures which are *performant*, *efficient* and with *fast* inference times is pivotal.
- Multi-objective problem with (potentially) **conflicting objectives**.
  - Optimizing all objectives simultaneously is infeasible.
  - Finding the **right trade-off** remains challenging.
- We also need efficient search methods for these kind of spaces.
  - Conventional blackbox methods, such as ES or BO, require multiple expensive evaluations.



# NAS in a world of ever growing models

- In an age of **large models**, finding architectures which are *performant*, *efficient* and with *fast* inference times is pivotal.
- Multi-objective problem with (potentially) **conflicting objectives**.
  - Optimizing all objectives simultaneously is infeasible.
  - Finding the **right trade-off** remains challenging.
- We also need efficient search methods for these kind of spaces.
  - Conventional blackbox methods, such as ES or BO, require multiple expensive evaluations.
- Multi-objective Differentiable NAS (**MODNAS**)
  - Leverages **hypernetworks** and **multiple gradient descent (MGD)** to profile the whole pareto front.
  - Scales across *multiple devices and objectives* with a **single search run**.



# Optimality in Multi-objective optimization

## Pareto optimality and Pareto front

MOO then seeks to find a set of Pareto-optimal solutions  $\alpha^*$  that jointly minimize  $\mathbf{L}(\alpha) \triangleq (\mathcal{L}^1(\alpha), \dots, \mathcal{L}^M(\alpha))$ :

$$\alpha^* \in \arg \min_{\alpha} \mathbf{L}(\alpha)$$



# Optimality in Multi-objective optimization

## Pareto optimality and Pareto front

MOO then seeks to find a set of Pareto-optimal solutions  $\alpha^*$  that jointly minimize  $\mathbf{L}(\alpha) \triangleq (\mathcal{L}^1(\alpha), \dots, \mathcal{L}^M(\alpha))$ :

$$\alpha^* \in \arg \min_{\alpha} \mathbf{L}(\alpha)$$

### Definition

**(Pareto Optimality):** A solution  $\alpha_2$  dominates  $\alpha_1$  iff  $\mathcal{L}^m(\alpha_2) \leq \mathcal{L}^m(\alpha_1)$ ,  $\forall m \in \{1, \dots, M\}$ , and  $\mathbf{L}(\alpha_1) \neq \mathbf{L}(\alpha_2)$ . In other words, a dominating solution has a lower loss value on at least one task and no higher loss value on any task. A solution  $\alpha^*$  is called *Pareto optimal* iff there exists no other solution dominating  $\alpha^*$ .



# Optimality in Multi-objective optimization

## Pareto optimality and Pareto front

MOO then seeks to find a set of Pareto-optimal solutions  $\alpha^*$  that jointly minimize  $\mathbf{L}(\alpha) \triangleq (\mathcal{L}^1(\alpha), \dots, \mathcal{L}^M(\alpha))$ :

$$\alpha^* \in \arg \min_{\alpha} \mathbf{L}(\alpha)$$

### Definition

**(Pareto Front):** The sets of Pareto optimal points and their function values are called *Pareto set* ( $\mathcal{P}_\alpha$ ) and *Pareto front* ( $\mathcal{P}_{\mathbf{L}} = \{\mathbf{L}(\alpha)_{\alpha \in \mathcal{P}_\alpha}\}$ ), respectively.

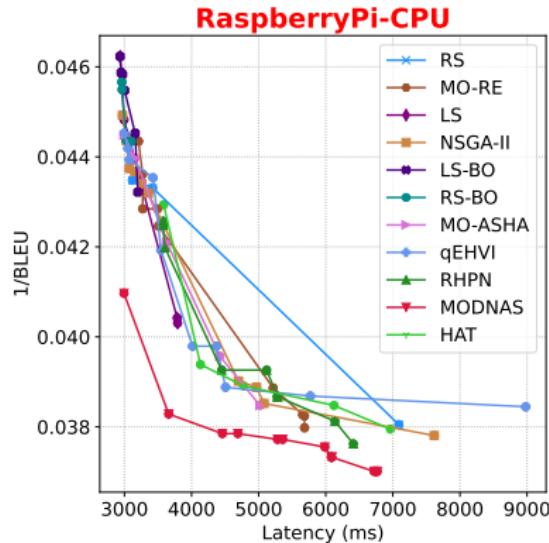


# Optimality in Multi-objective optimization

## Pareto optimality and Pareto front

MOO then seeks to find a set of Pareto-optimal solutions  $\alpha^*$  that jointly minimize  $\mathbf{L}(\alpha) \triangleq (\mathcal{L}^1(\alpha), \dots, \mathcal{L}^M(\alpha))$ :

$$\alpha^* \in \arg \min_{\alpha} \mathbf{L}(\alpha)$$



# Problem Formulation

Multi-objective NAS as bi-level optimization

Assuming we have **T hardware devices** (target functions) and **M objectives** (e.g. accuracy, latency, energy usage, etc.), the Pareto set  $\mathcal{P}_{\alpha_t}$  of the multi-objective NAS problem is obtained by solving the following **bi-level optimization** problem:

$$\begin{aligned} & \arg \min_{\alpha} \mathbf{L}_t^{valid}(\mathbf{w}^*(\alpha), \alpha) \\ \text{s.t. } & \mathbf{w}^*(\alpha) = \arg \min_{\mathbf{w}} \mathbf{L}_t^{train}(\mathbf{w}, \alpha), \end{aligned}$$

where the  $M$ -dimensional loss vector

$\mathbf{L}_t(\mathbf{w}^*, \alpha) \triangleq (\mathcal{L}_t^1(\mathbf{w}^*, \alpha), \dots, \mathcal{L}_t^M(\mathbf{w}^*, \alpha))$  is evaluated  $\forall t \in \{1, \dots, T\}$ .



# Problem Formulation

Multi-objective NAS as bi-level optimization

Assuming we have **T hardware devices** (target functions) and **M objectives** (e.g. accuracy, latency, energy usage, etc.), the Pareto set  $\mathcal{P}_{\alpha_t}$  of the multi-objective NAS problem is obtained by solving the following **bi-level optimization** problem:

$$\begin{aligned} & \arg \min_{\alpha} \mathbf{L}_t^{valid}(\mathbf{w}^*(\alpha), \alpha) \\ \text{s.t. } & \mathbf{w}^*(\alpha) = \arg \min_{\mathbf{w}} \mathbf{L}_t^{train}(\mathbf{w}, \alpha), \end{aligned}$$

where the  $M$ -dimensional loss vector

$\mathbf{L}_t(\mathbf{w}^*, \alpha) \triangleq (\mathcal{L}_t^1(\mathbf{w}^*, \alpha), \dots, \mathcal{L}_t^M(\mathbf{w}^*, \alpha))$  is evaluated  $\forall t \in \{1, \dots, T\}$ .

- Still **expensive**...
  - Need to run the search  $T$  times.
  - Cannot be solved exactly due to the expensive lower problem.



- ① MetaPredictor: regression model to predict cheap-to-evaluate hardware objectives (e.g. latency, energy usage, etc.)
- ② Supernetwork: proxy to approximate the lower level best response function  $w^*(\alpha)$
- ③ MetaHypernetwork: hypernetwork to generate unnormalized architectural distribution conditioned on preference vectors and hardware device type
- ④ Architect: samples from the architectural distribution discrete architectures



- For the cheap-to-evaluate hardware objectives, such as latency, energy consumption.

- For the cheap-to-evaluate hardware objectives, such as latency, energy consumption.
- A parametric regression model (e.g. MLP)  $p_\theta^m(\alpha, d_t^m) : \mathcal{A} \times \mathcal{H} \rightarrow \mathbb{R}$ .

- For the cheap-to-evaluate hardware objectives, such as latency, energy consumption.
- A parametric regression model (e.g. MLP)  $p_\theta^m(\alpha, d_t^m) : \mathcal{A} \times \mathcal{H} \rightarrow \mathbb{R}$ .
- We use the same predictors as in [1] and optimize the MSE loss:

$$\min_{\theta} \mathbb{E}_{\alpha \sim \mathcal{A}, t \sim [T]} (y_t^m - p_\theta^m(\alpha, d_t^m))^2$$

- For the cheap-to-evaluate hardware objectives, such as latency, energy consumption.
- A parametric regression model (e.g. MLP)  $p_\theta^m(\alpha, d_t^m) : \mathcal{A} \times \mathcal{H} \rightarrow \mathbb{R}$ .
- We use the same predictors as in [1] and optimize the MSE loss:

$$\min_{\theta} \mathbb{E}_{\alpha \sim \mathcal{A}, t \sim [T]} (y_t^m - p_\theta^m(\alpha, d_t^m))^2$$

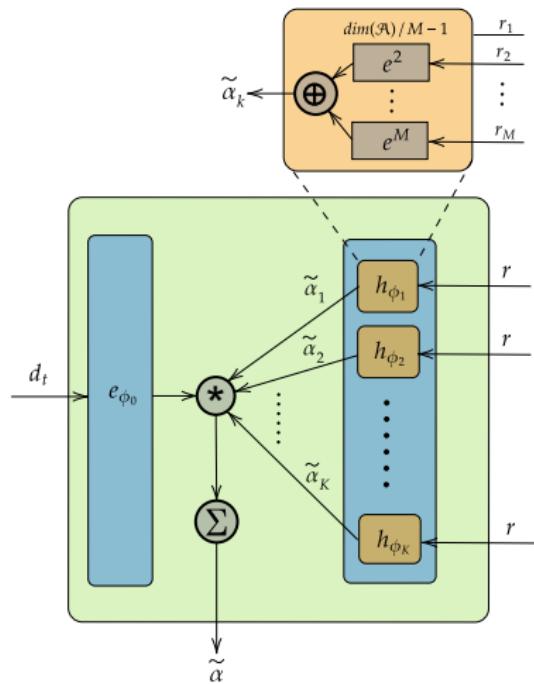
- Use  $\mathcal{L}_t^m(\cdot, \alpha_\Phi) = p_\theta^m(\alpha_\Phi, d_t^m)$  as the objective function.
  - During the search we freeze and do not update further the MetaPredictor parameters  $\theta$ .



# MODNAS

## MetaHypernetwork

- We use a hypernetwork  $H_\Phi(\mathbf{r}, d_t)$  that takes as input a **device embedding**  $d_t$  and a **preference vector**  $\mathbf{r} \in \mathbb{R}^M$  to yield an architecture distribution  $\tilde{\alpha}$ .
  - Just a forward pass to generate an architecture.
  - Scalable across different hardware devices.



# MODNAS

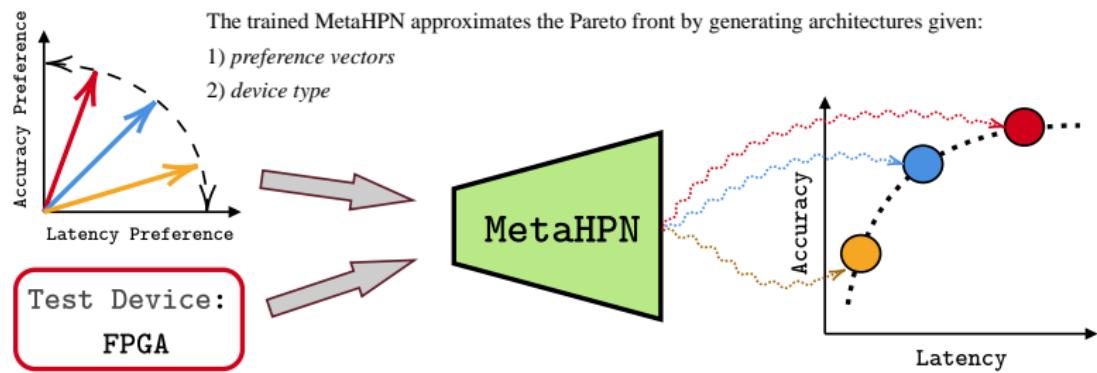
## Linear Scalarization

Using the **preference vector  $r$**  to create a linear scalarization of  $\mathbf{L}_t$  and the MetaHypernetwork to model the architectural distribution across  $T$  devices, the bi-level problem reduces to:

$$\arg \min_{\Phi} \mathbb{E}_{r \sim \mathcal{S}} [r^T \mathbf{L}_t^{valid}(\mathbf{w}^*(\alpha_\Phi), \alpha_\Phi)]$$

$$s.t. \quad \mathbf{w}^*(\alpha_\Phi) = \arg \min_{\mathbf{w}} \mathbb{E}_{r \sim \mathcal{S}} [r^T \mathbf{L}_t^{train}(\mathbf{w}, \alpha_\Phi)],$$

where  $r^T \mathbf{L}_t(\cdot, \alpha_\Phi) = \sum_{m=1}^M r_m \mathcal{L}_t^m(\cdot, \alpha_\Phi)$  is the scalarized loss for device  $t$ .



# MODNAS

## Linear Scalarization

Using the **preference vector**  $\mathbf{r}$  to create a linear scalarization of  $\mathbf{L}_t$  and the MetaHypernetwork to model the architectural distribution across  $T$  devices, the bi-level problem reduces to:

$$\begin{aligned} & \arg \min_{\Phi} \mathbb{E}_{\mathbf{r} \sim \mathcal{S}} [\mathbf{r}^T \mathbf{L}_t^{valid}(\mathbf{w}^*(\alpha_\Phi), \alpha_\Phi)] \\ \text{s.t. } & \mathbf{w}^*(\alpha_\Phi) = \arg \min_{\mathbf{w}} \mathbb{E}_{\mathbf{r} \sim \mathcal{S}} [\mathbf{r}^T \mathbf{L}_t^{train}(\mathbf{w}, \alpha_\Phi)], \end{aligned}$$

where  $\mathbf{r}^T \mathbf{L}_t(\cdot, \alpha_\Phi) = \sum_{m=1}^M r_m \mathcal{L}_t^m(\cdot, \alpha_\Phi)$  is the scalarized loss for device  $t$ .

- Conditioning the MetaHypernetwork on the hardware embeddings allows us to generate architectures on new test devices without extra finetuning or meta-learning steps.



# MODNAS

## Linear Scalarization

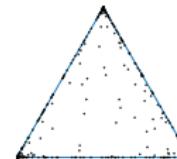
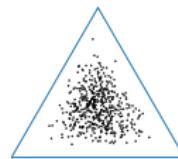
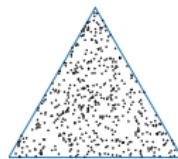
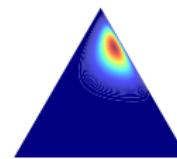
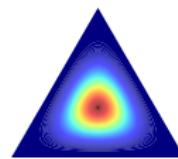
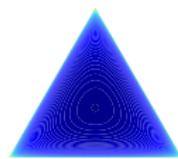
We sample the preference vector  $r$  from a Dirichlet distribution with concentration parameters  $\beta_1, \dots, \beta_M = 1$ .

$$\beta = (0.999, 0.999, 0.999)$$

$$\beta = (5.000, 5.000, 5.000)$$

$$\beta = (2.000, 5.000, 15.000)$$

$$\beta = (0.100, 0.100, 0.100)$$



# MODNAS

## Optimizing the MetaHypernetwork with MGD

- Multiple Gradient Descent (MGD) seeks to simultaneously optimize the MetaHypernetwork parameters (shared across all devices)  $\Phi \leftarrow \Phi - \xi g_{\Phi}^*$ , where:  
$$g_{\Phi}^* = \sum_{t=1}^T \gamma_t^* g_{\Phi}^t$$



# MODNAS

## Optimizing the MetaHypernetwork with MGD

- Multiple Gradient Descent (MGD) seeks to simultaneously optimize the MetaHypernetwork parameters (shared across all devices)  $\Phi \leftarrow \Phi - \xi g_{\Phi}^*$ , where:  
$$g_{\Phi}^* = \sum_{t=1}^T \gamma_t^* g_{\Phi}^t$$
- What are the optimal  $\gamma_t^*$ ?

$$\min_{\gamma_1, \dots, \gamma_T} \left\{ \left\| \sum_{t=1}^T \gamma_t g_{\Phi}^t \right\|_2^2 \mid \sum_{t=1}^T \gamma_t = 1, \gamma_t \geq 0, \forall t \right\}.$$



# MODNAS

## Optimizing the MetaHypernetwork with MGD

- Multiple Gradient Descent (MGD) seeks to simultaneously optimize the MetaHypernetwork parameters (shared across all devices)  $\Phi \leftarrow \Phi - \xi g_{\Phi}^*$ , where:  
$$g_{\Phi}^* = \sum_{t=1}^T \gamma_t^* g_{\Phi}^t$$
- What are the optimal  $\gamma_t^*$ ?

$$\min_{\gamma_1, \dots, \gamma_T} \left\{ \left\| \sum_{t=1}^T \gamma_t g_{\Phi}^t \right\|_2^2 \mid \sum_{t=1}^T \gamma_t = 1, \gamma_t \geq 0, \forall t \right\}.$$

- $T = 2$ :

$$\gamma^* = \max \left( \min \left( \frac{(g_{\Phi}^2 - g_{\Phi}^1)^T g_{\Phi}^2}{\|g_{\Phi}^1 - g_{\Phi}^2\|_2^2}, 1 \right), 0 \right)$$

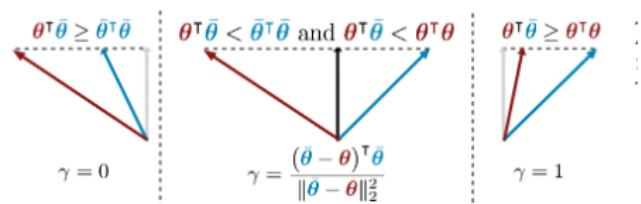


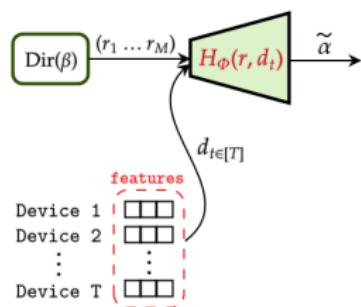
Figure 1: Visualisation of the min-norm point in the convex hull of two points ( $\min_{\gamma \in [0,1]} \|\gamma \theta + (1 - \gamma) \bar{\theta}\|_2^2$ ). As the geometry suggests, the solution is either an edge case or a perpendicular vector.

- $T > 2$ :

Frank-Wolfe solver [Jaggi, 2013]

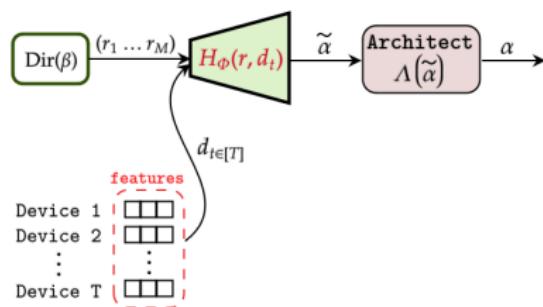
# MODNAS

All pieces together



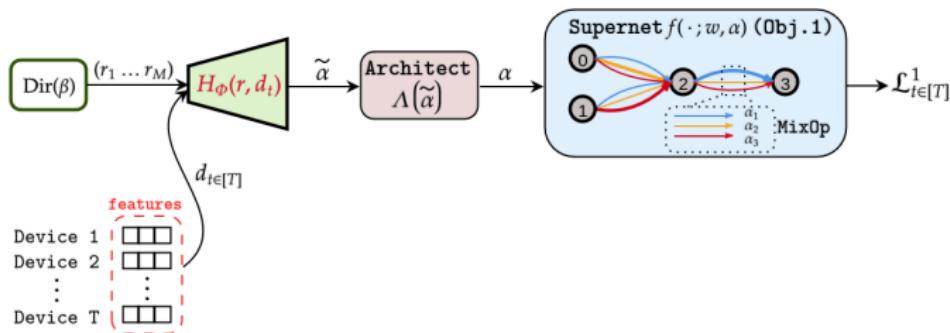
# MODNAS

All pieces together



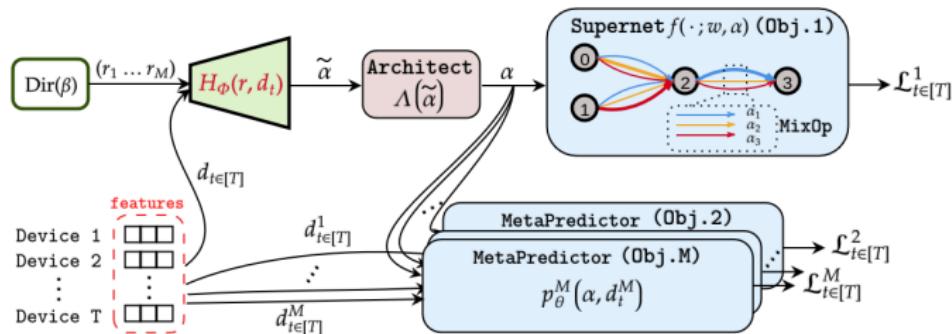
# MODNAS

All pieces together



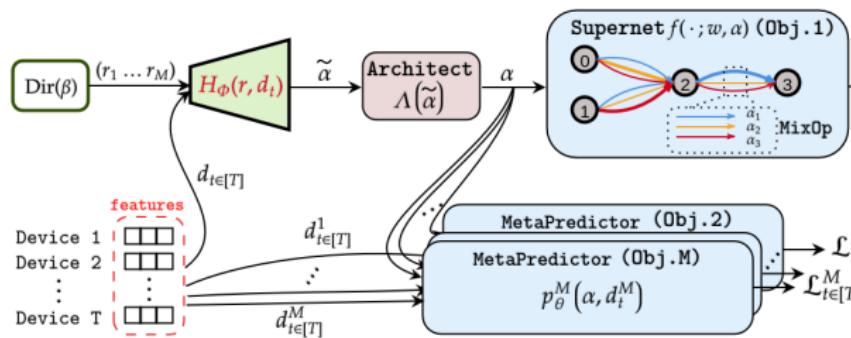
# MODNAS

All pieces together



# MODNAS

All pieces together



$$\begin{aligned} g_\Phi^1 &= \nabla_\Phi (r_1 \mathcal{L}_1^1 + r_2 \mathcal{L}_2^1 + \dots + r_M \mathcal{L}_M^1) \\ g_\Phi^T &= \nabla_\Phi (r_1 \mathcal{L}_1^T + r_2 \mathcal{L}_2^T + \dots + r_M \mathcal{L}_M^T) \\ \text{Update } \Phi \text{ using SGD: } g_\Phi^* &= \sum_{t=1}^T \gamma_t g_\Phi^t \end{aligned}$$

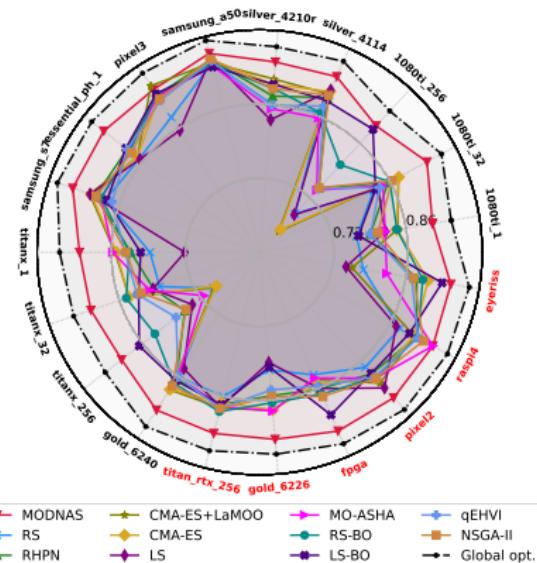
$r_m$  : scalarizations     $f(\cdot; w, \alpha)$  : supernet  
 $d_t^m$  : hw embedd.     $p_\theta^m(\cdot)$  : predictor  
 $\mathcal{L}_t^m$  : loss                       $H_\Phi$  : hypernet  
 $\alpha, \tilde{\alpha}$  : arch param



# Experimental results

Simultaneous Pareto Set Learning across 19 devices on NB201

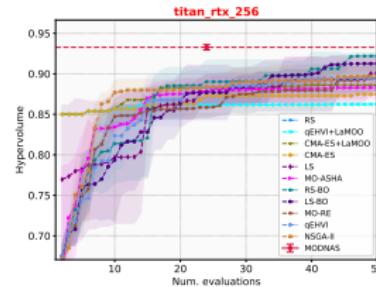
- **Metric:** Hypervolume (HV) indicator.
- **Baselines:**
  - Random baselines
  - Evolutionary strategies
  - Bayesian Optimization
- **Evaluation:** Sample 24 preference vectors and get the MAP architecture from the MetaHypernetwork output for each of them.



# Experimental results

MetaHypernetwork update schemes: robustness of MGD

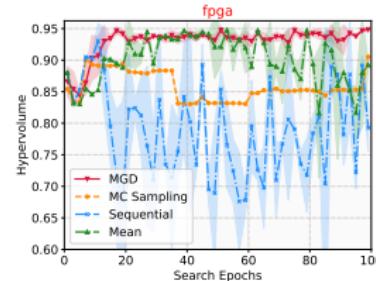
- **Metric:** Hypervolume (HV) indicator over time.



- **Baselines:**

- Mean grad update
- Sequential grad updates
- Grad samples updates

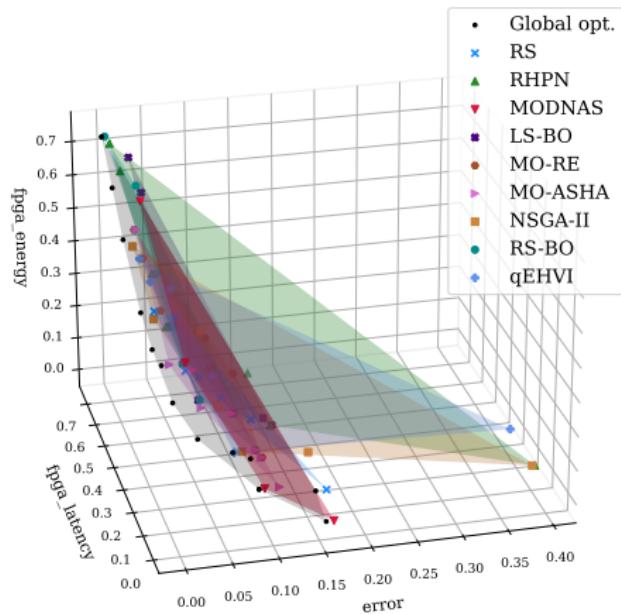
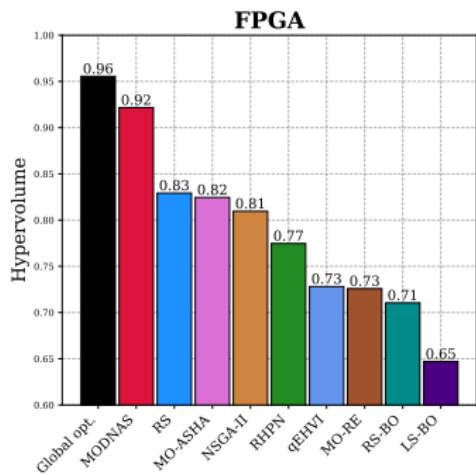
- **Evaluation:** Sample 24 preference vectors and get the MAP architecture from the MetaHypernetwork output for each of them.



# Experimental results

## Scalability to 3 objectives

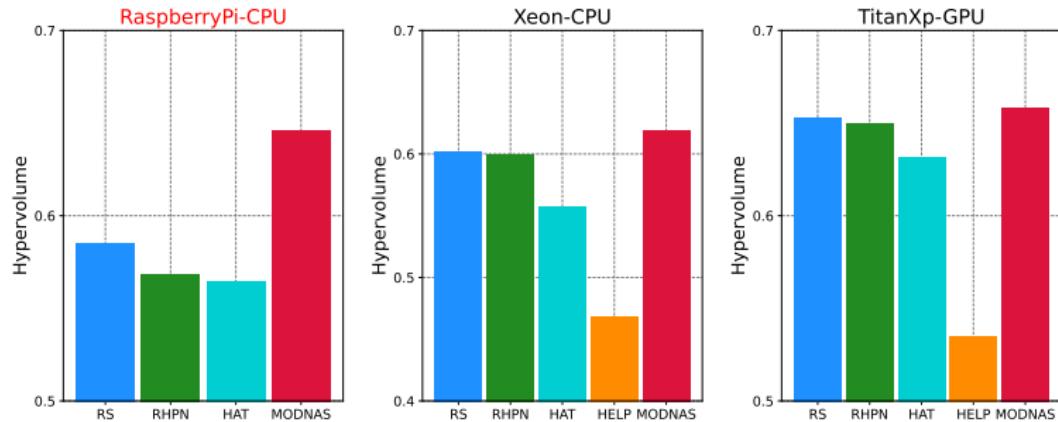
- Optimize for *latency*, *energy usage* and *accuracy* simultaneously across devices.



# Experimental results

## Pareto front profiling on Transformer Spaces

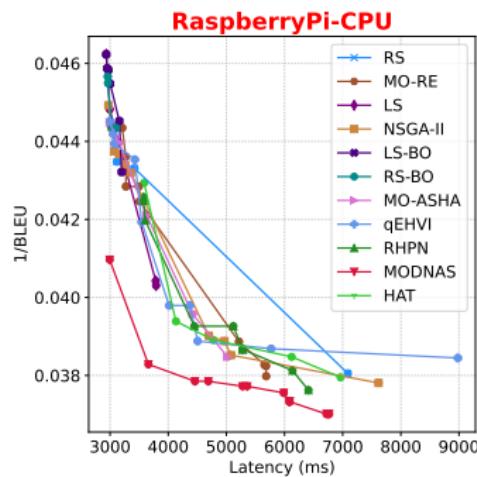
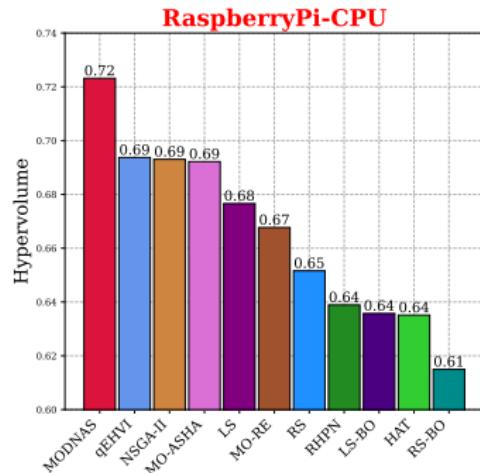
- We run MODNAS on the **Hardware-Aware Transformer (HAT)** [Wang et al. 2020] search space on the WMT'14 En-De machine translation task.
- **Search costs:** 6 days on 8 NVidia RTX A6000



# Experimental results

## Pareto front profiling on Transformer Spaces

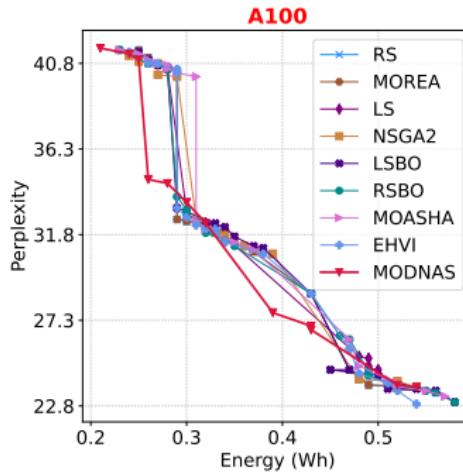
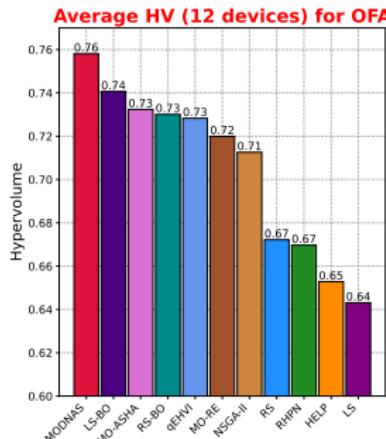
- We run MODNAS on the **Hardware-Aware Transformer (HAT)** [Wang et al. 2020] search space on the WMT'14 En-De machine translation task.
- Search costs:** 6 days on 8 NVidia RTX A6000



# Experimental results

Efficient MOO on ImageNet-1k and OpenWebText starting from Pretrained Supernetworks

- We use the **Once-for-All (OFA)** [Cai et al. 2020] pretrained supernet on ImageNet and run MODNAS for 1 day on 8 GPUs.
- We also use **HW-GPT-Bench** texttt[Sukthanker et al. 2024] to run MODNAS on a GPT-2 search space.
- **Higher HV** compared to baselines



# Summary and future directions

- MODNAS can **profile the pareto front** of various objective spaces.



## Summary and future directions

- MODNAS can **profile the pareto front** of various objective spaces.
- Via a **hypernetwork** and **MGD**, MODNAS can optimize simultaneously across many devices (up to 19) and multiple objectives (up to 3).



## Summary and future directions

- MODNAS can **profile the pareto front** of various objective spaces.
- Via a **hypernetwork** and **MGD**, MODNAS can optimize simultaneously across many devices (up to 19) and multiple objectives (up to 3).
- We show **improved hypervolume on test devices** across various spaces, tasks and datasets, without additional fine-tuning and with less search costs.



# Summary and future directions

- MODNAS can **profile the pareto front** of various objective spaces.
- Via a **hypernetwork** and **MGD**, MODNAS can optimize simultaneously across many devices (up to 19) and multiple objectives (up to 3).
- We show **improved hypervolume on test devices** across various spaces, tasks and datasets, without additional fine-tuning and with less search costs.
- <https://arxiv.org/pdf/2402.18213>

**In the future:**



## Summary and future directions

- MODNAS can **profile the pareto front** of various objective spaces.
- Via a **hypernetwork** and **MGD**, MODNAS can optimize simultaneously across many devices (up to 19) and multiple objectives (up to 3).
- We show **improved hypervolume on test devices** across various spaces, tasks and datasets, without additional fine-tuning and with less search costs.
- <https://arxiv.org/pdf/2402.18213>

### In the future:

- Extend MODNAS to work in the Few-shot NAS settings with subspace partitions.



## Summary and future directions

- MODNAS can **profile the pareto front** of various objective spaces.
- Via a **hypernetwork** and **MGD**, MODNAS can optimize simultaneously across many devices (up to 19) and multiple objectives (up to 3).
- We show **improved hypervolume on test devices** across various spaces, tasks and datasets, without additional fine-tuning and with less search costs.
- <https://arxiv.org/pdf/2402.18213>

### In the future:

- Extend MODNAS to work in the Few-shot NAS settings with subspace partitions.
- More control on the preference vector sampler during search.



Thank you for your attention.  
Questions?