Efficient Continuous Pareto Exploration in Multi-Task Learning

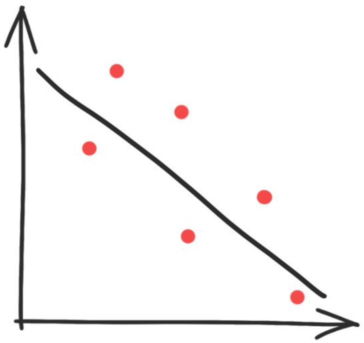
Pingchuan Ma*, Tao Du*, Wojciech Matusik
MIT CSAIL

CSAIL

ICML | 2020

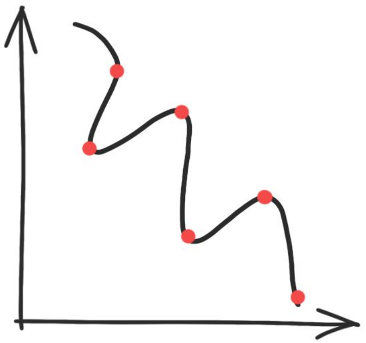
Motivation

Multiple objectives are common in machine learning.



More bias
Less variance

V.S.



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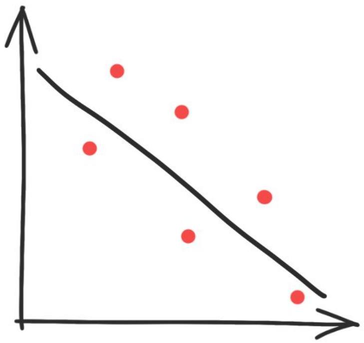

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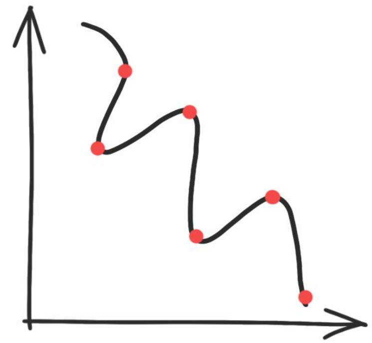

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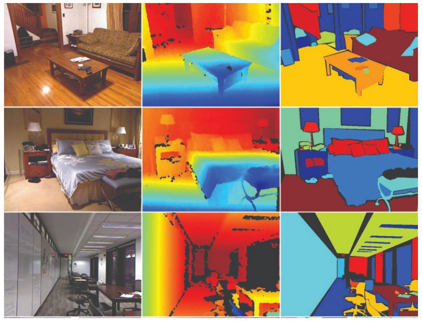
Label(s): Cat, Dog, Duck

Multi-Label

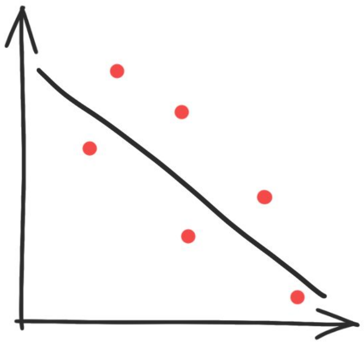


Modal(s): Image, Depth, Segmentation

Multimodal

Motivation

...but objectives often conflict with each other!



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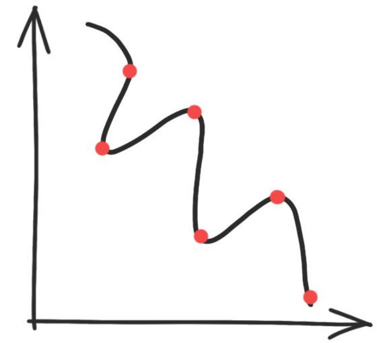

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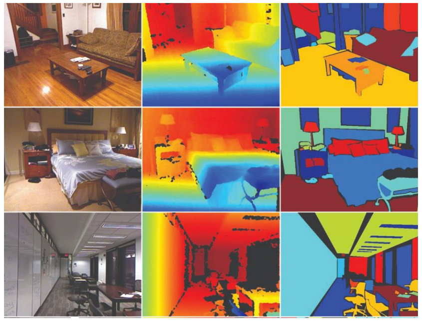

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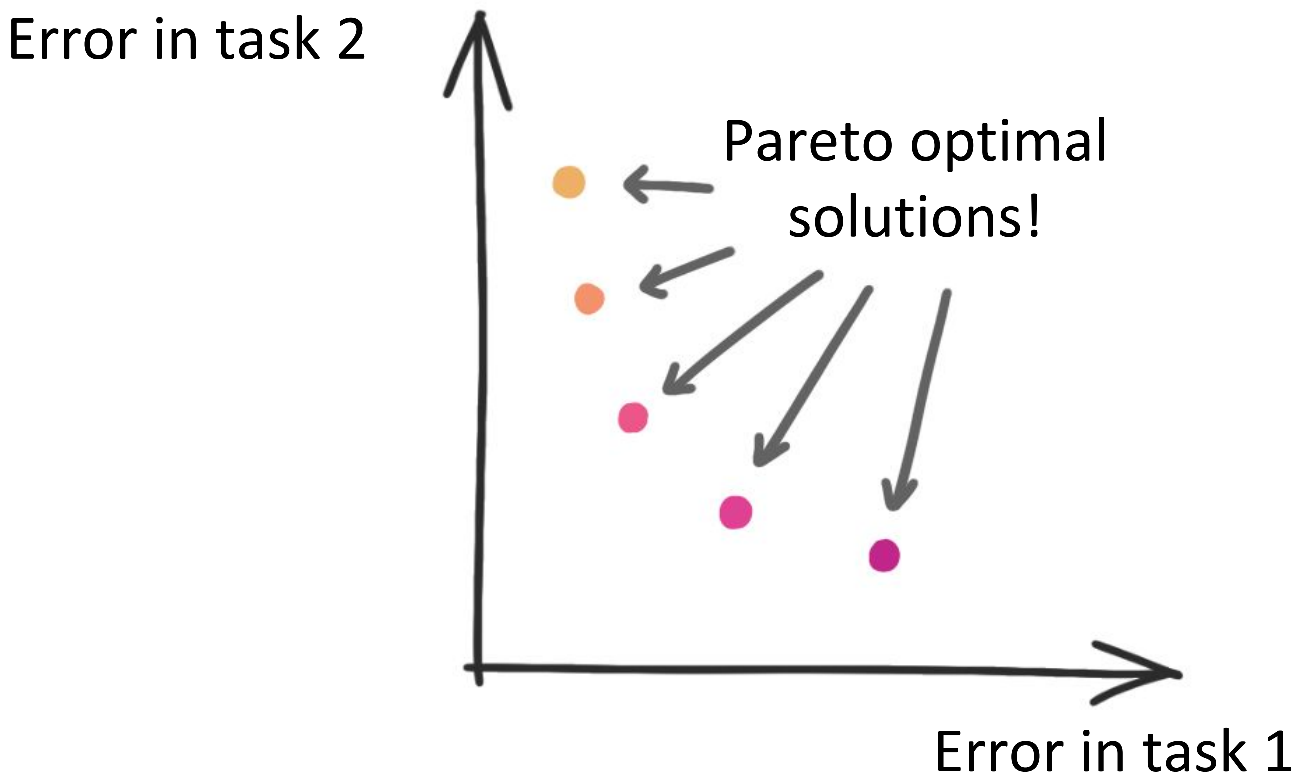
Multimodal

Motivation

This is characterized by the concept of Pareto optimality.



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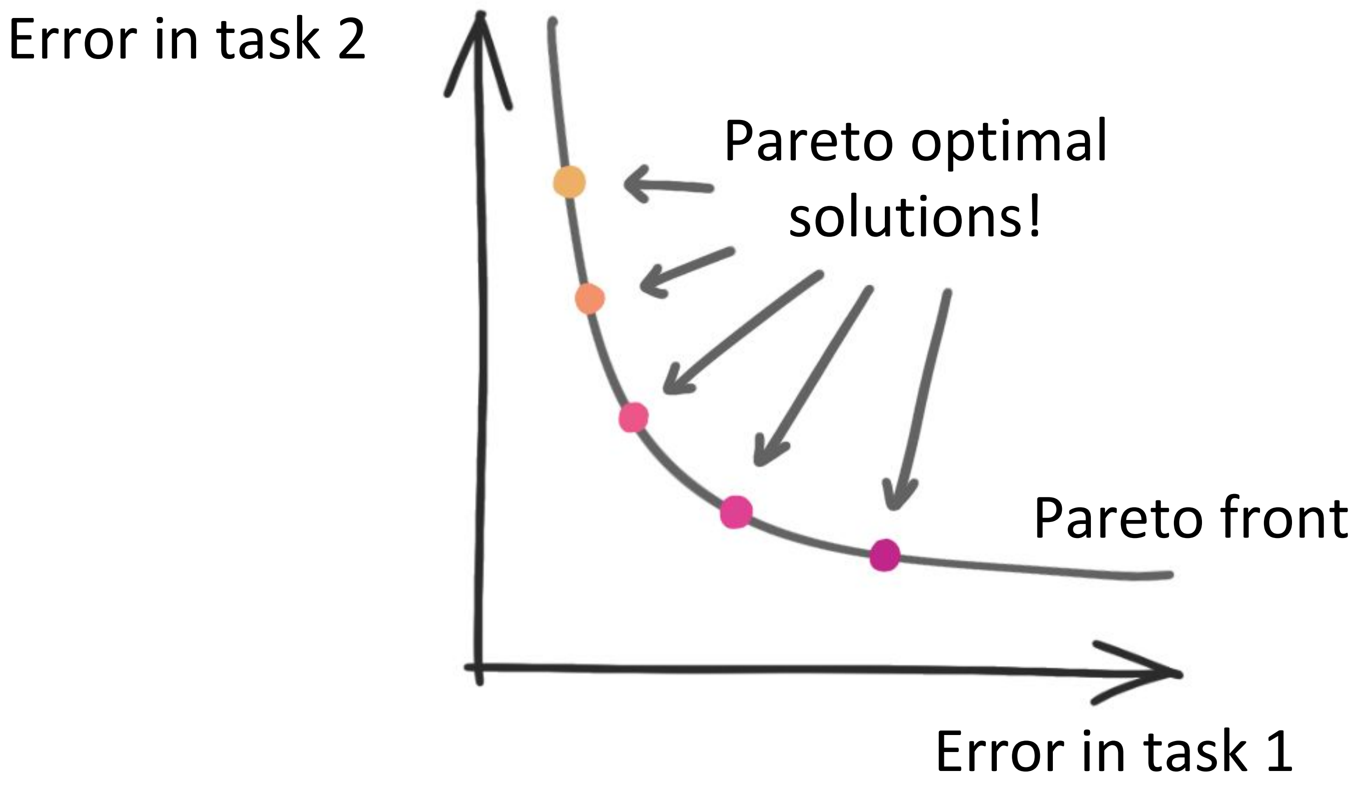


Related work

Multi-objective optimization

ıere exist vectors $\lambda \in \mathbb{R}^m$ and $\alpha \in \mathbb{R}^k$, wit
= 1, such that

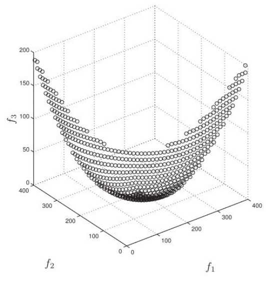
$$\sum_{i=1}^{k} \alpha_i \nabla f_i(x^*) + \sum_{j=1}^{m} \lambda_j \nabla h_j(x^*) = 0,$$

$$h_i(x^*) = 0, \qquad i = 1, \ldots, m.$$

define the scalar-valued function

$$g_\alpha : \mathbb{R}^n \to \mathbb{R}, \qquad x \mapsto g_\alpha(x) := \sum_{i=1}^{k} \alpha_i f_i(x),$$

Hillermeier
2001



Martin & Schutze
2018

	Solution type	Problem size
Hillermeier 01 Martin & Schutze 18	Continuous	Small

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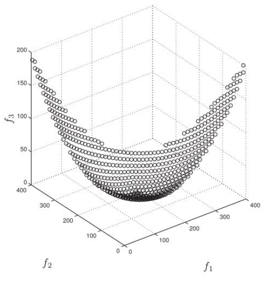
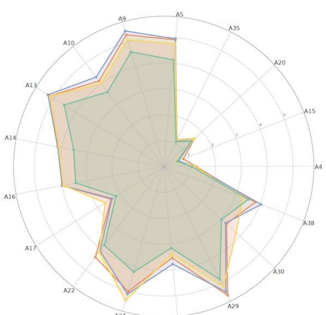
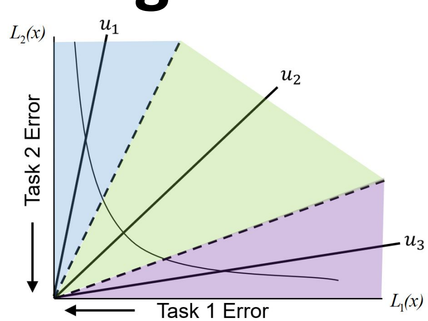


Martin & Schutze
2018

Multi-task learning



Sener & Koltun
2018



Lin et al.
2019

	Solution type	Problem size
Hillermeier 01 Martin & Schutze 18	Continuous	Small
Chen et al. 18 Kendall et al. 18 Sener & Koltun 18	Single discrete	Large
Lin et al. 19	Multiple discrete	Large

Contributions

- We presented the first method to discover **continuous approximations** to Pareto fronts for **large deep-learning problems**.

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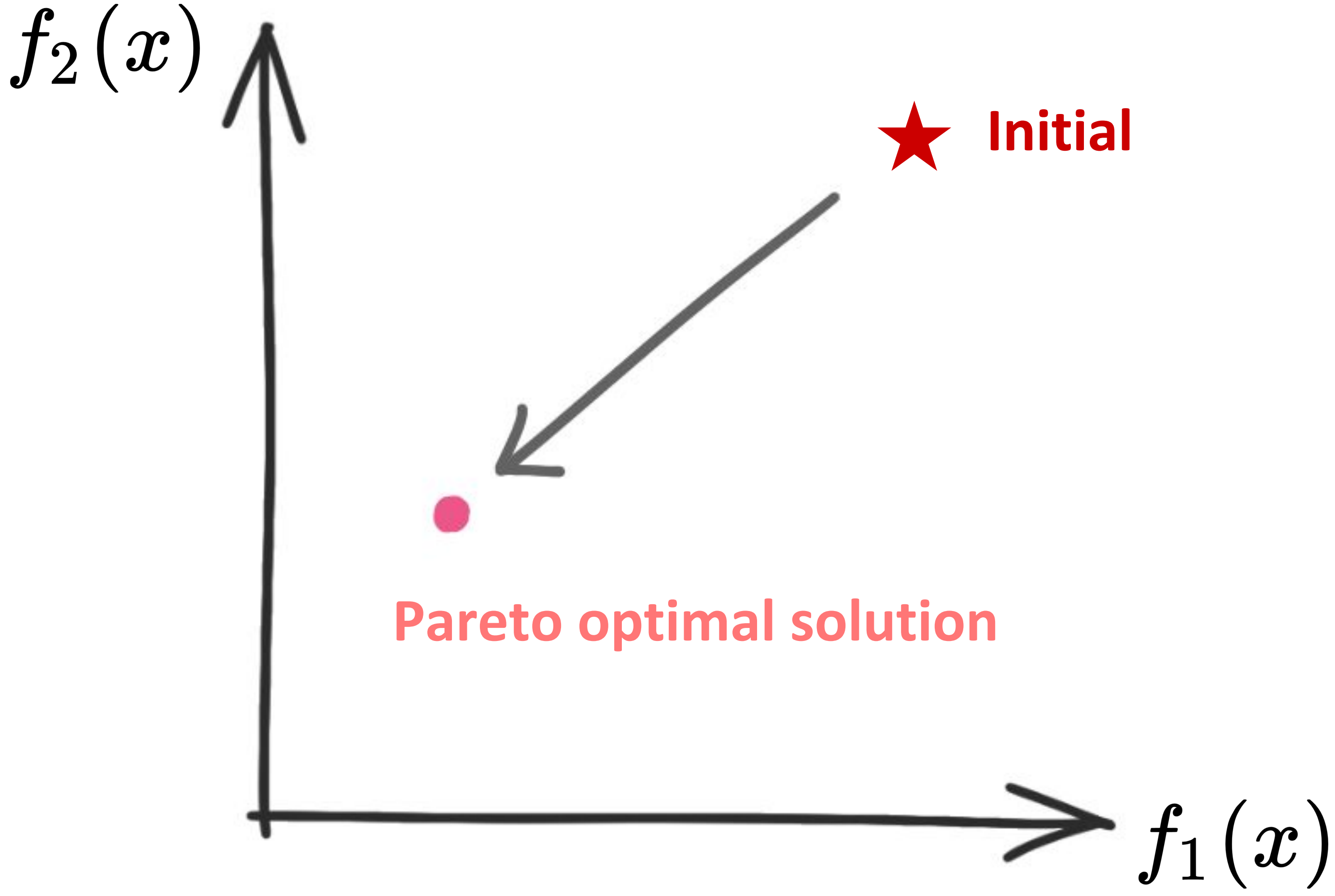
Ours	Continuous	Large

Method overview



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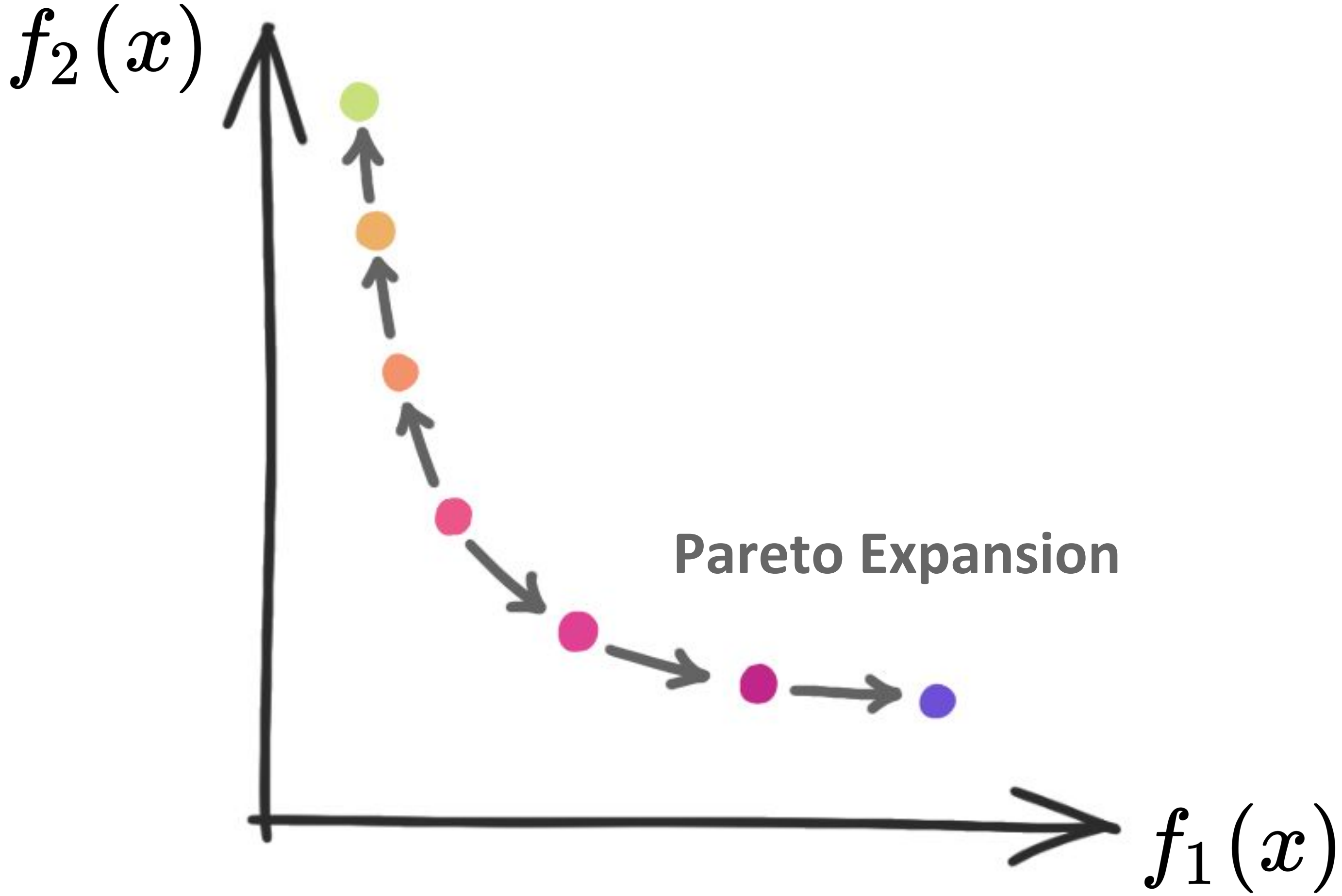

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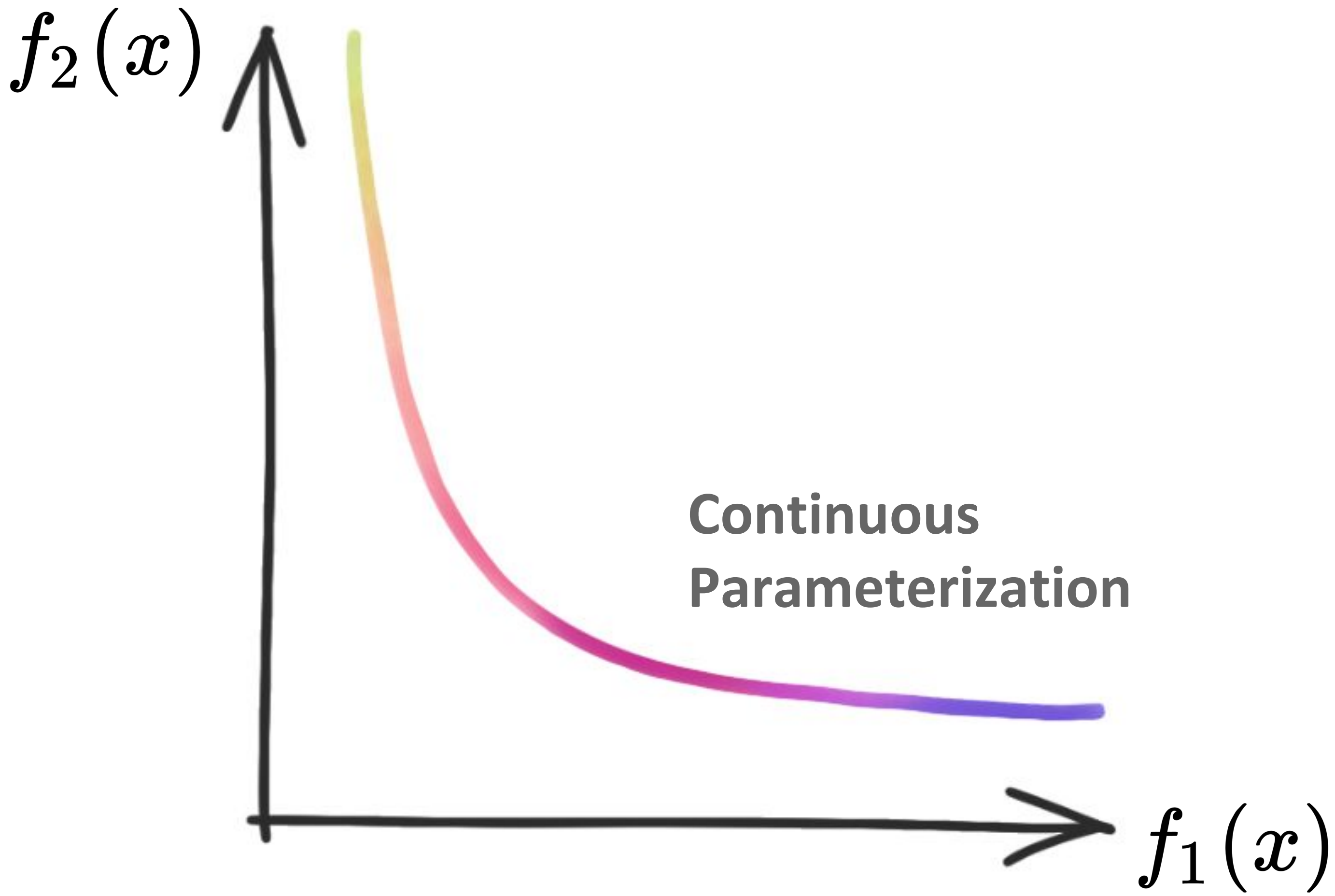

Challenges

- **The most efficient direction for expansion is unknown.**
  - How to recover the Pareto front from one solution?
- **Deep-learning parameter space has large dimensions.**
  - How to scale the method up for large-size problems?
- **Pareto solutions are discrete.**
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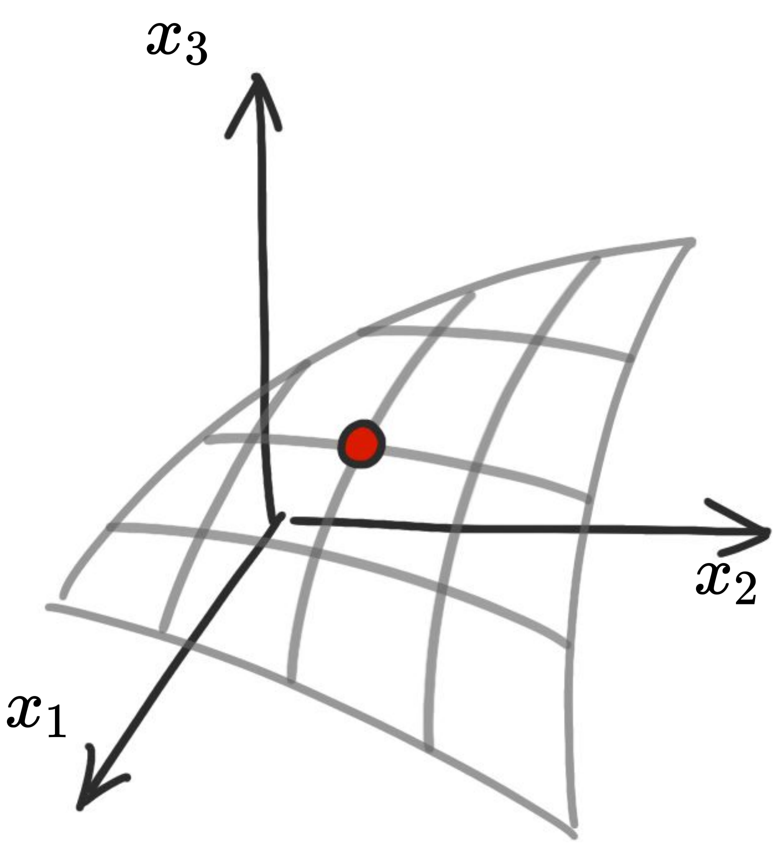
Efficient Pareto-front expansion



- **Necessary conditions**

$$\sum \alpha_i \nabla f_i(\mathbf{x}^*) = 0$$
$$\text{s.t. } \sum \alpha_i = 1,\ \boldsymbol{\alpha} \geq \mathbf{0}$$

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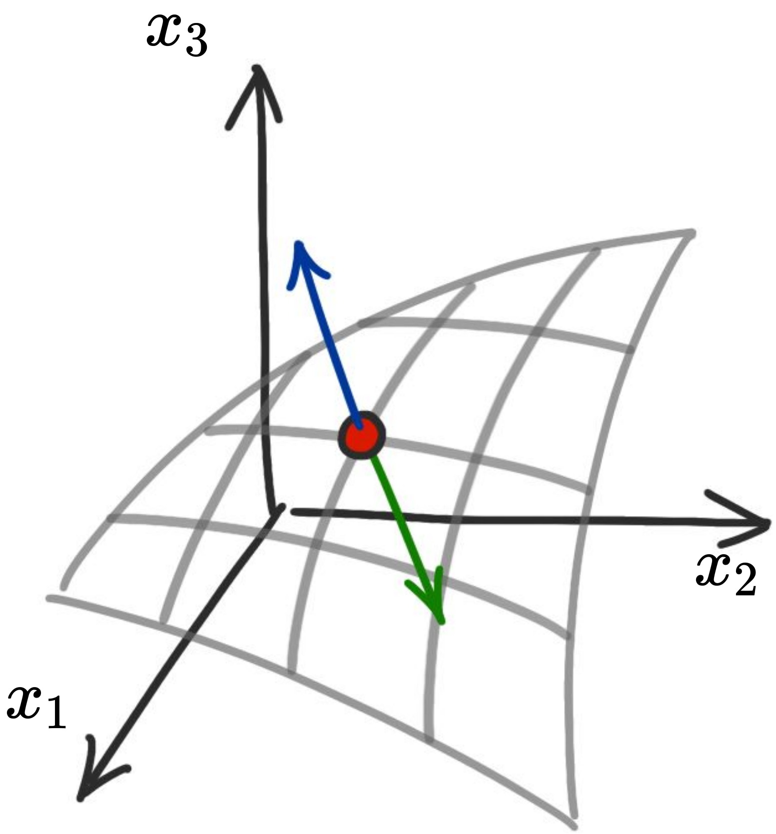

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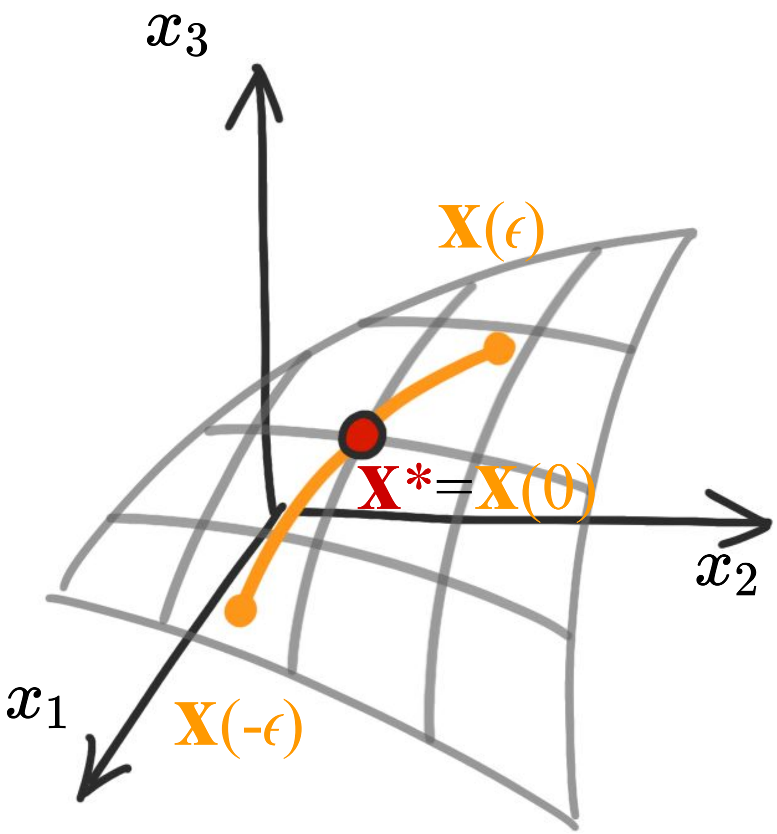
- Specifically:

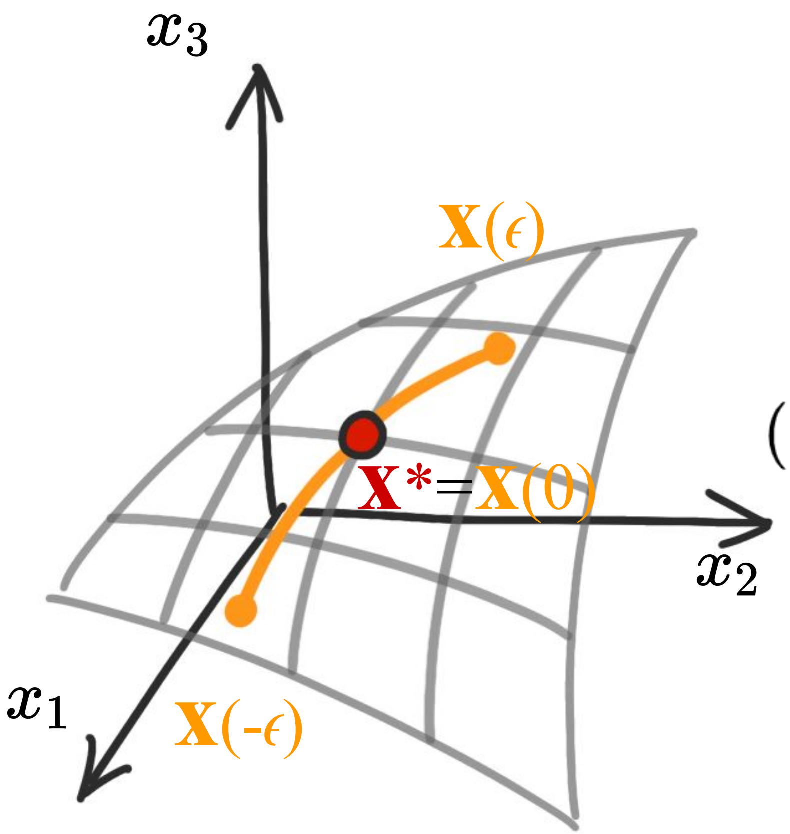
$$\alpha_1 \nabla f_1(\mathbf{x}^*) + \alpha_2 \nabla f_2(\mathbf{x}^*) = 0$$

Efficient Pareto-front expansion



$$\forall -\epsilon \leq t \leq \epsilon$$
$$\sum \alpha_i(t) \nabla f_i(\mathbf{x}(t)) = \mathbf{0}$$

Efficient Pareto-front expansion



$$\forall -\epsilon \leq t \leq \epsilon$$

$$\frac{d}{dt} \sum \alpha_i(t) \nabla f_i(\mathbf{x}(t)) = \mathbf{0}$$

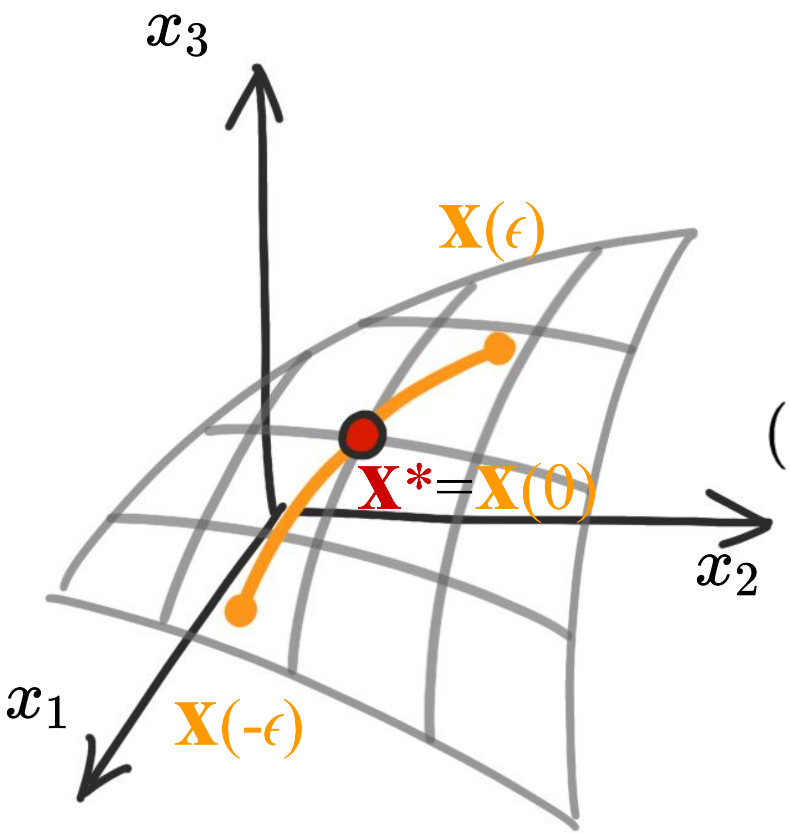
Differentiate ↓ Evaluate at $t = 0$

$$\left(\sum \alpha_i \nabla^2 f_i\right) x'(0) = -\sum \alpha_i' \nabla f_i\left(x(0)\right)$$

||

Our interest

Efficient Pareto-front expansion



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↓

$$\mathbf{H}v = \nabla \mathbf{f} \beta \in \text{colspan}\{\nabla f_i\}$$

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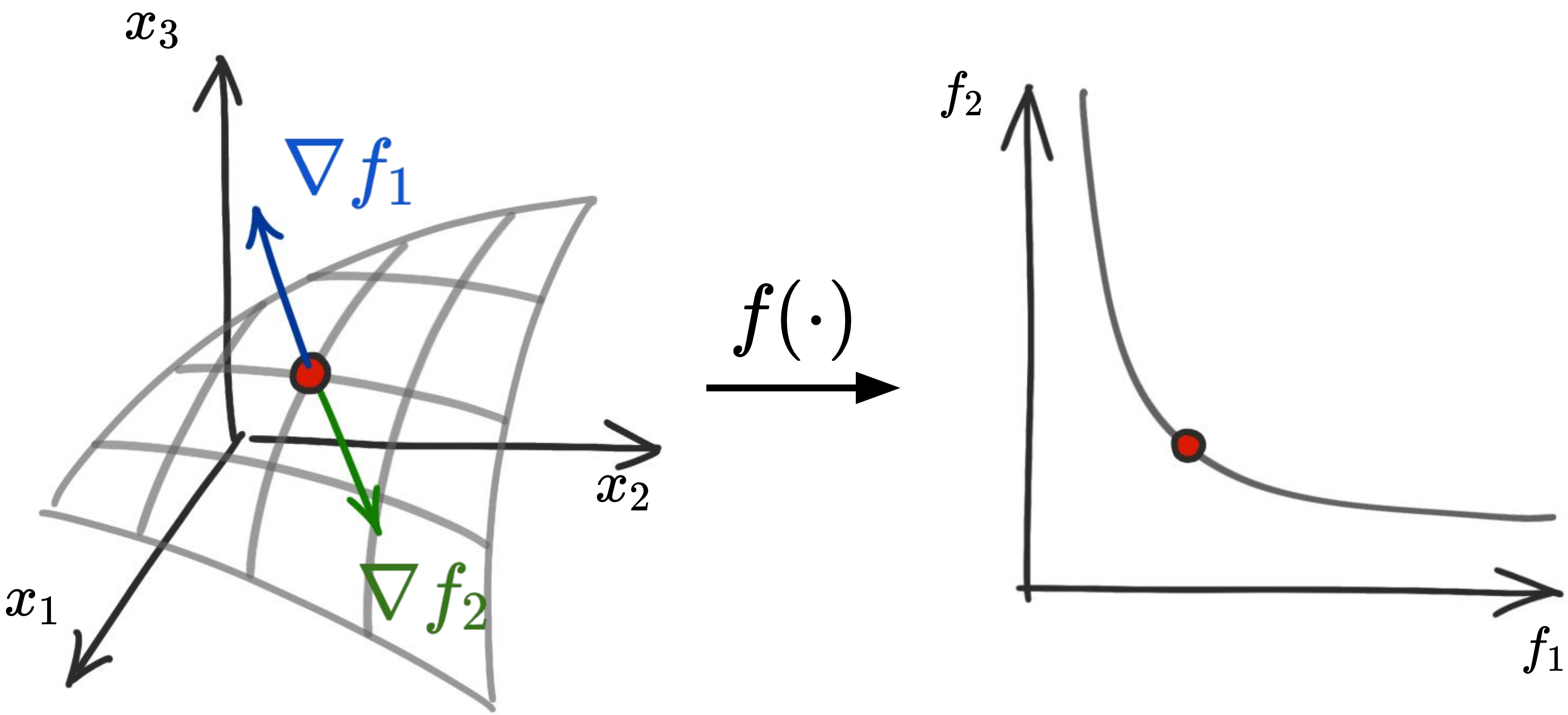

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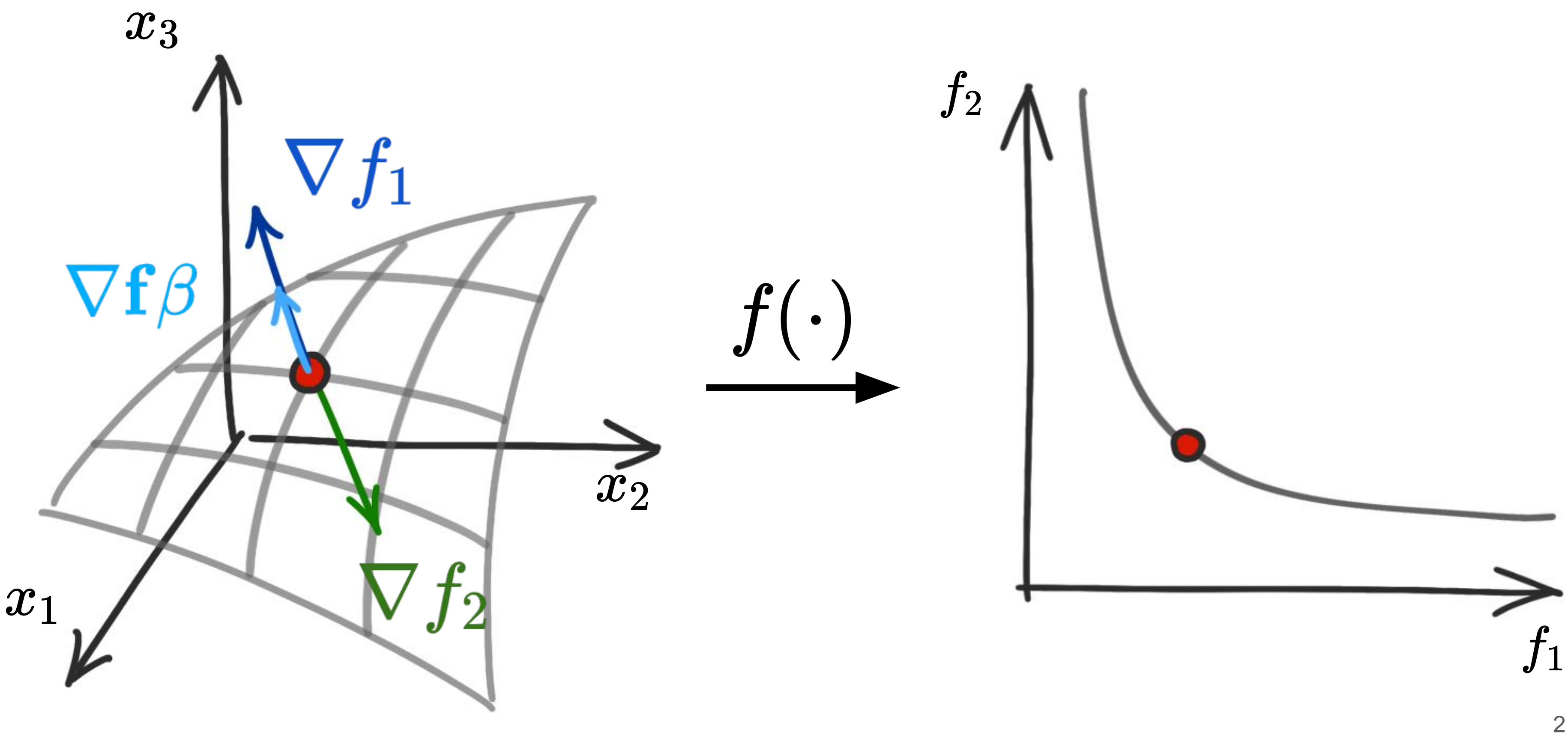

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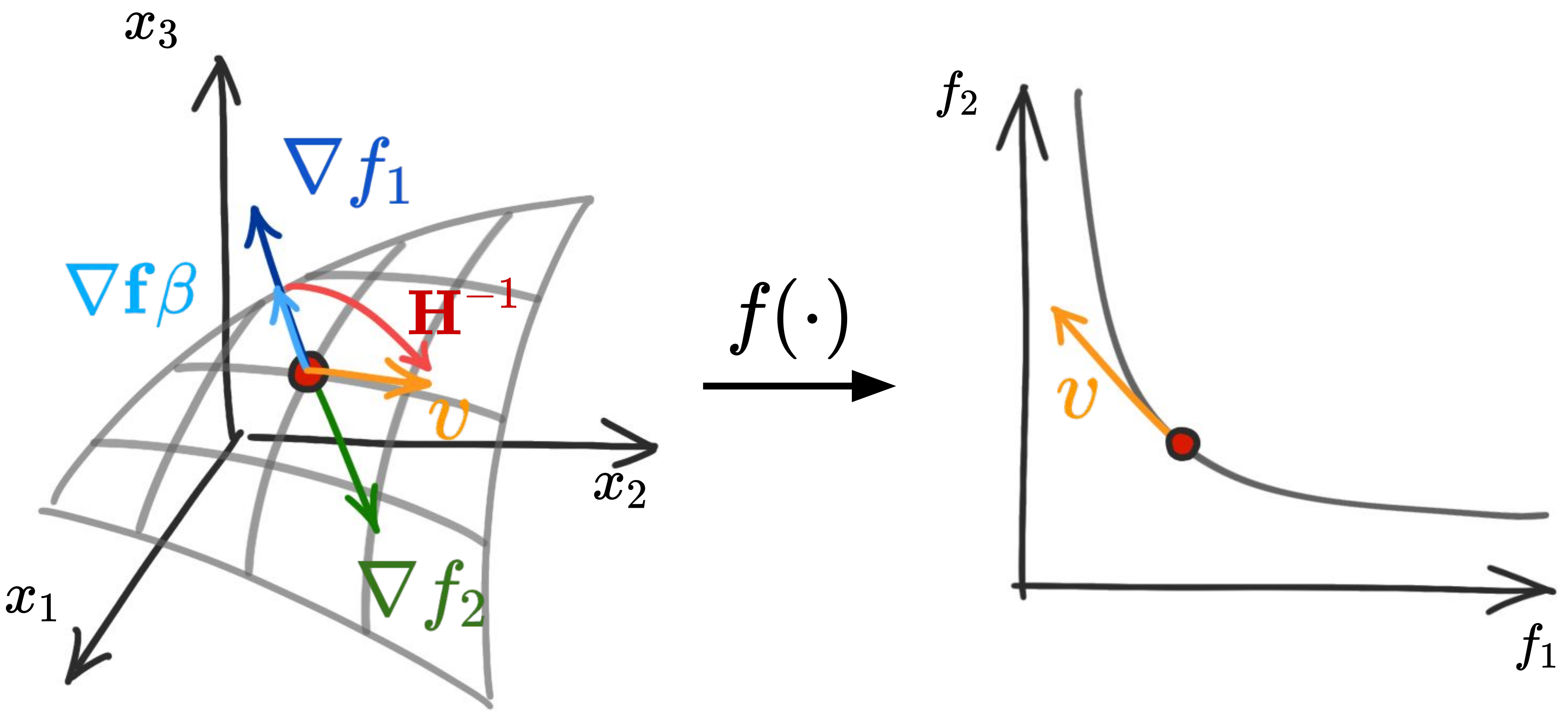

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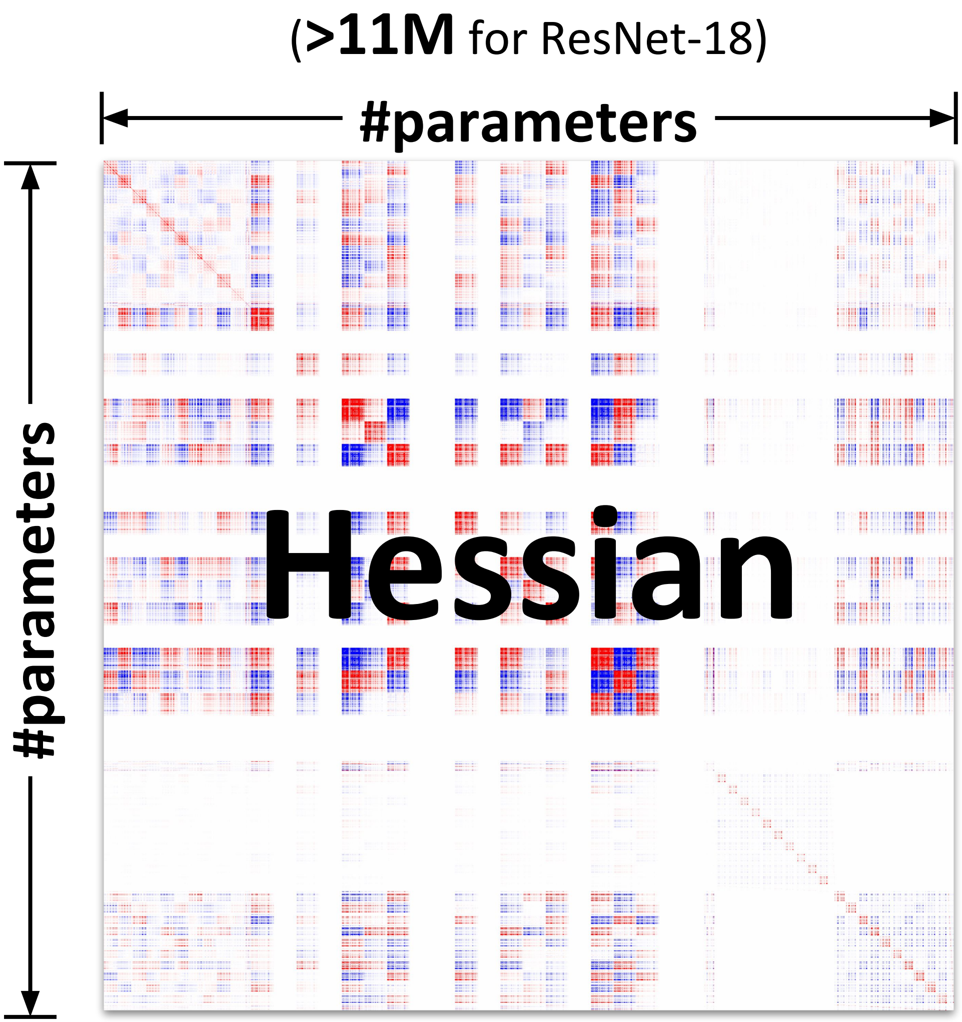
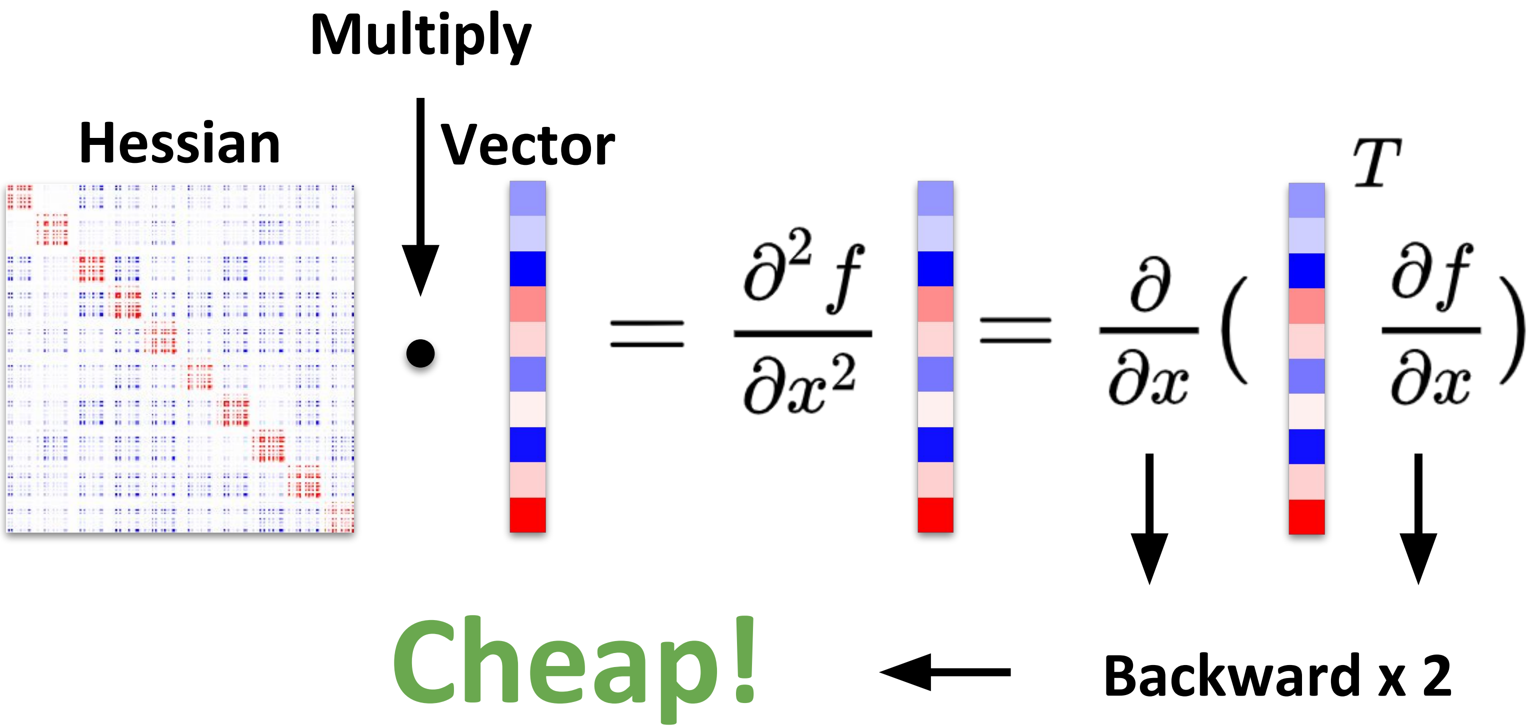
Scaling it up: the large Hessian issue



- Hessian: **HUGE** (>100 T elements to compute or store)
- Hessian^{-1} : **EXPENSIVE**

Scaling it up: Hessian-vector products (HVP)



$$\frac{\partial^2 f}{\partial x^2}\, v = \frac{\partial}{\partial x}\left(v^T \frac{\partial f}{\partial x} \right)$$

Scaling it up: HVP implementation

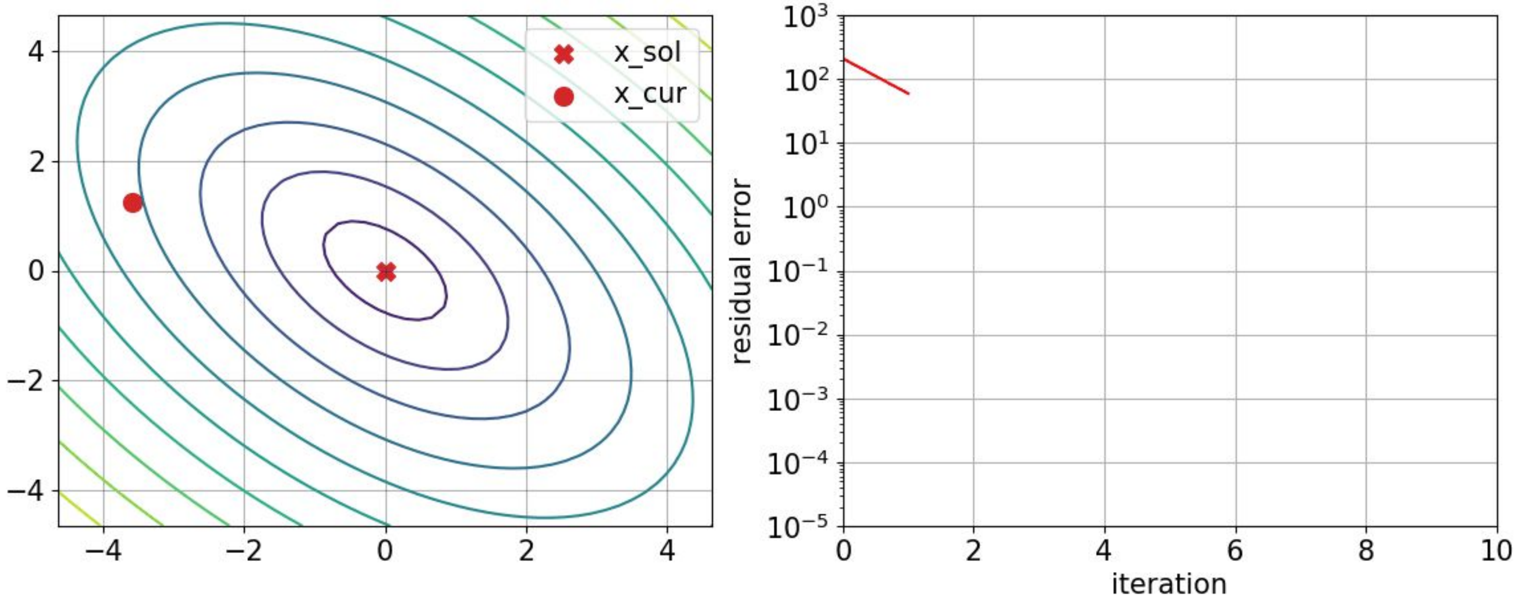
```
def hessian_vector_product(loss, network, v):

    params = network.parameters()

    jacobian = torch.autograd.grad(loss, params, create_graph=True)

    dot = v @ nn.utils.parameters_to_vector(jacobian)

    hvp = torch.autograd.grad(dot, params)

    return nn.utils.parameters_to_vector(hvp)
```

$$\mathbf{H}v = \frac{\partial^2 f}{\partial x^2} v = \frac{\partial}{\partial x}\boxed{\left(v^T \boxed{\frac{\partial f}{\partial x}}\right)}$$

Scaling it up: Krylov subspace method

Key features

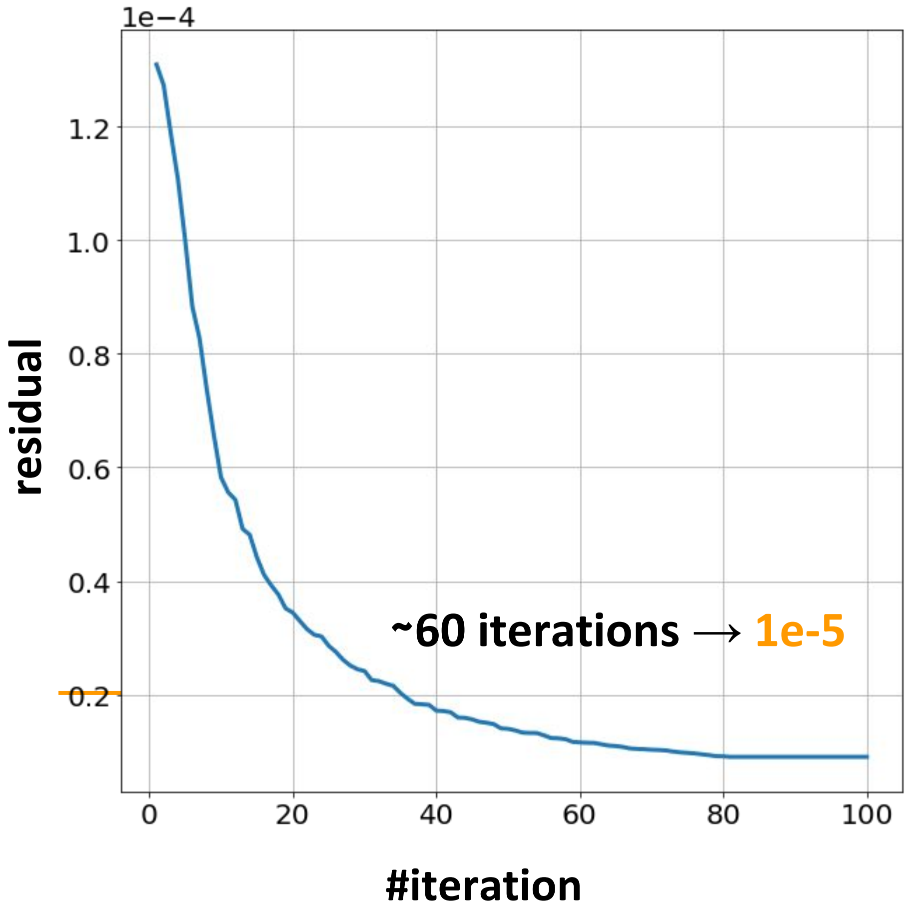
- ❑ More iterations (bounded by the matrix size) = better solutions
- ❑ Each iterations requires matrix-vector products only!



Applying the Conjugate Gradient method to solve a linear system of size 100 x 100.

Scaling it up: Implementation

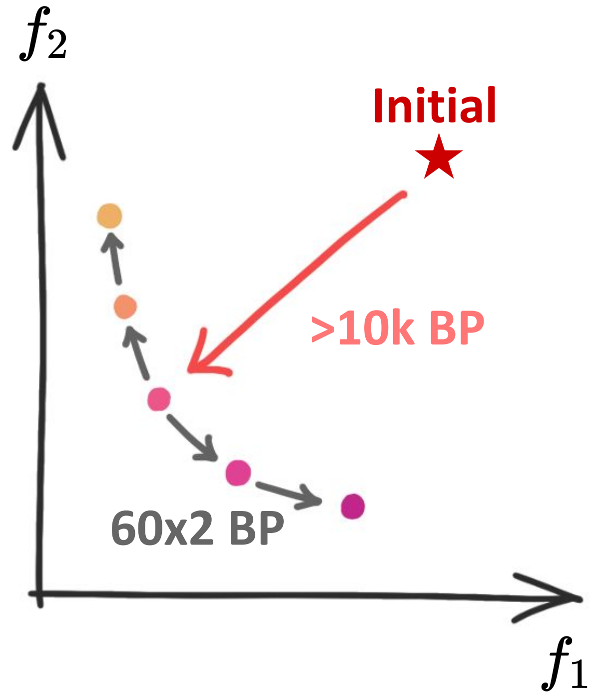
Deep-learning benchmark test (Hessian size = 1500^2)



- Lower residual is better
- Quick convergence compared with the matrix size

Scaling it up: Implication

Are 60 iterations cheap?



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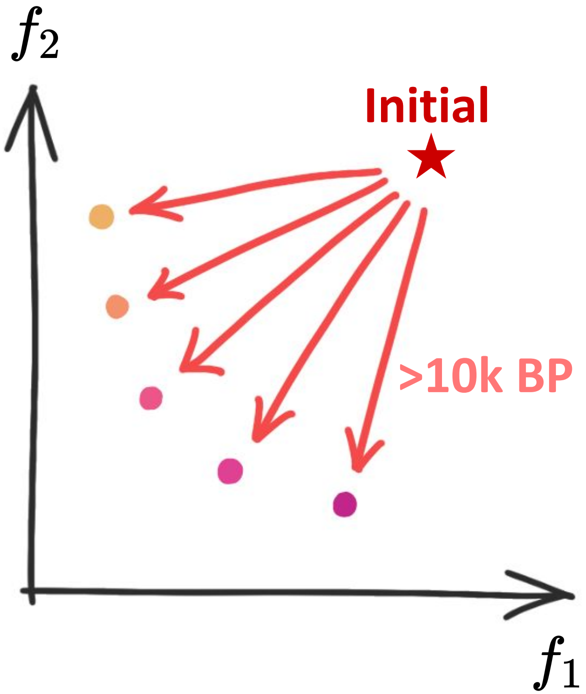

Zero-order method
(re-training)

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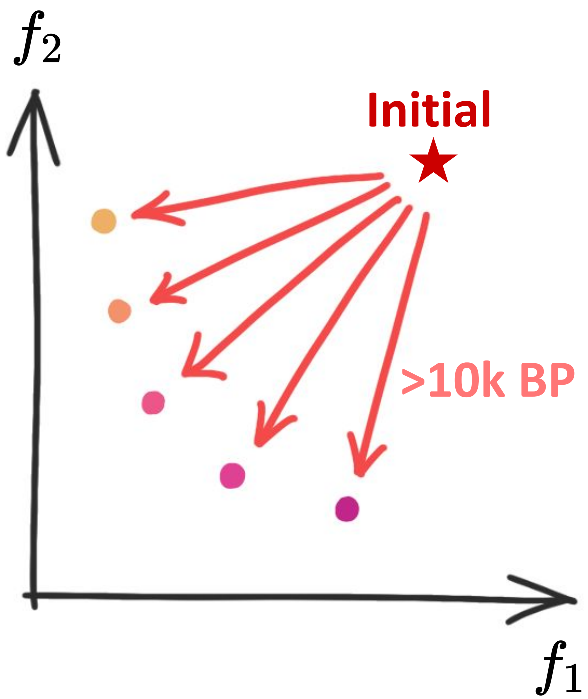

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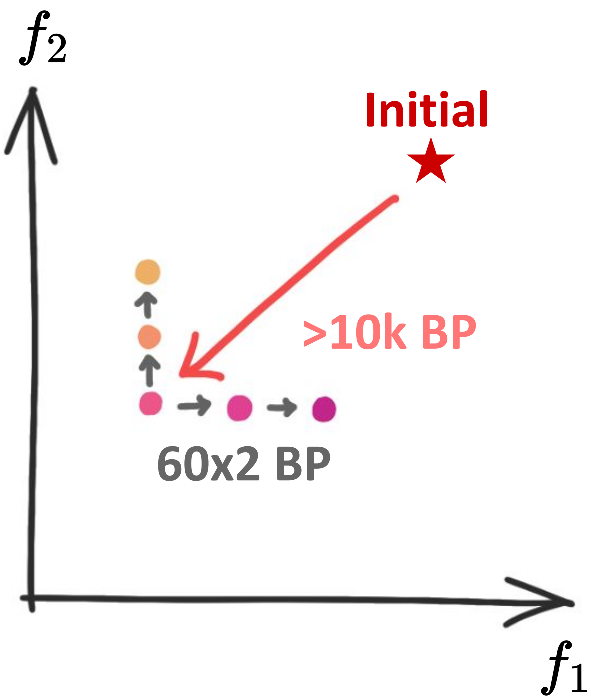
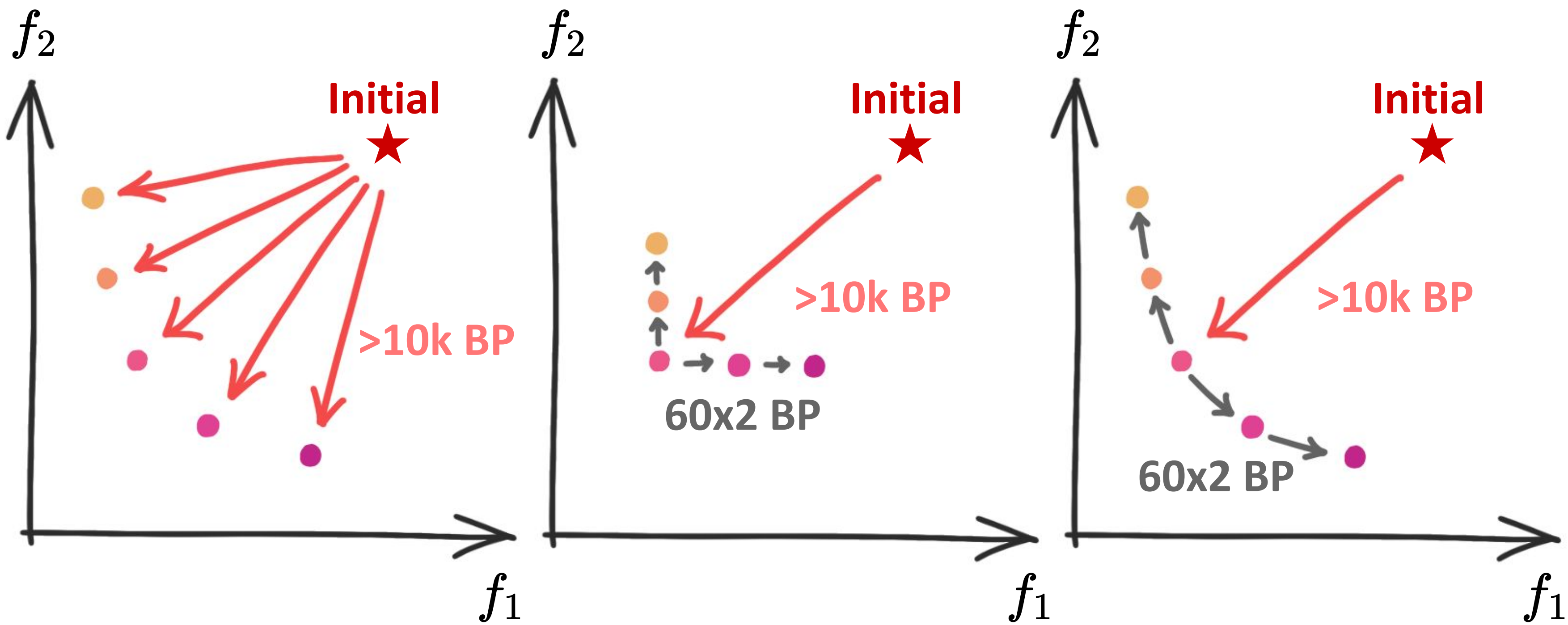


First-order method
(warm-start SGD)

Scaling it up: Implication

Are 60 iterations cheap? Yes!



Zero-order method (re-training)	First-order method (warm-start SGD)	**Second-order method (ours)**

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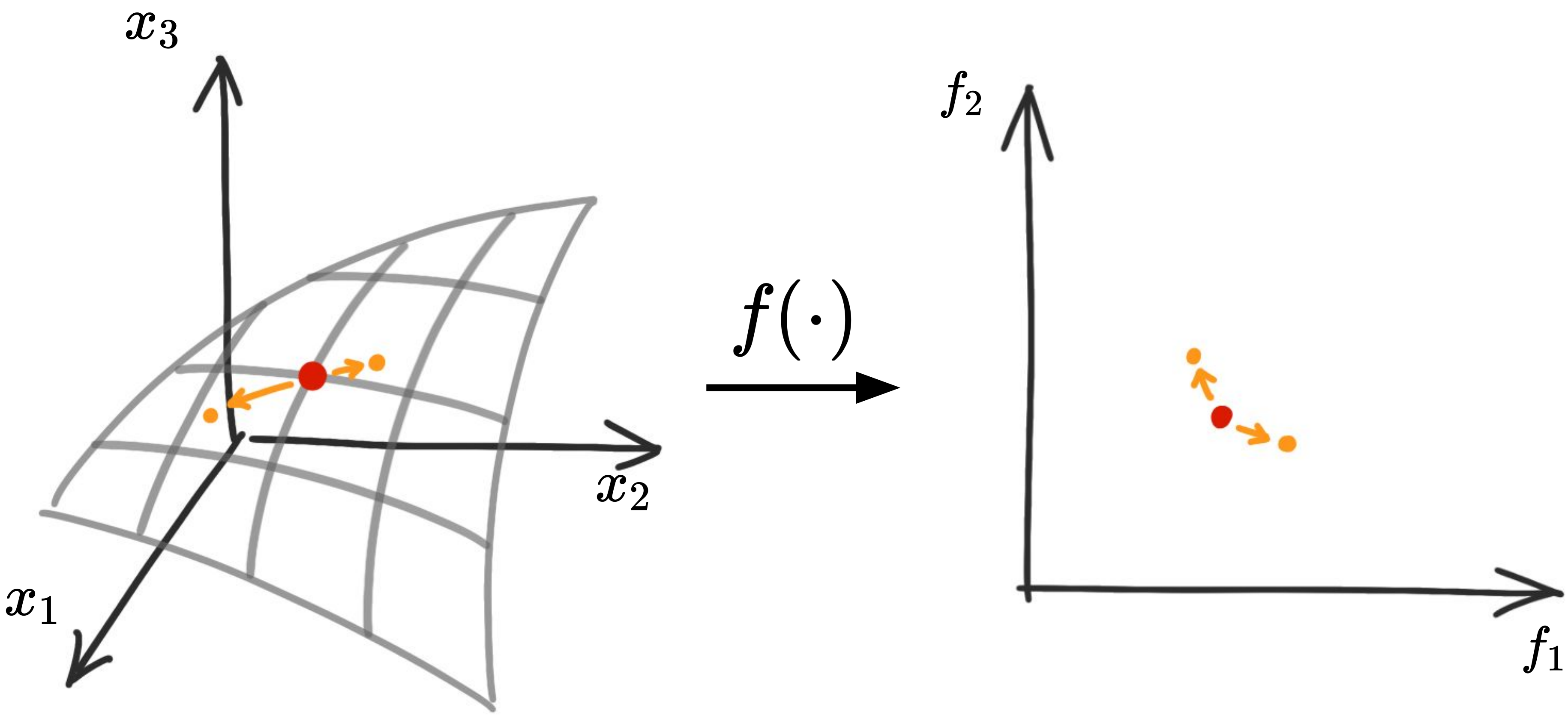
Challenges: Continuous Parameterization

Grow some solutions.



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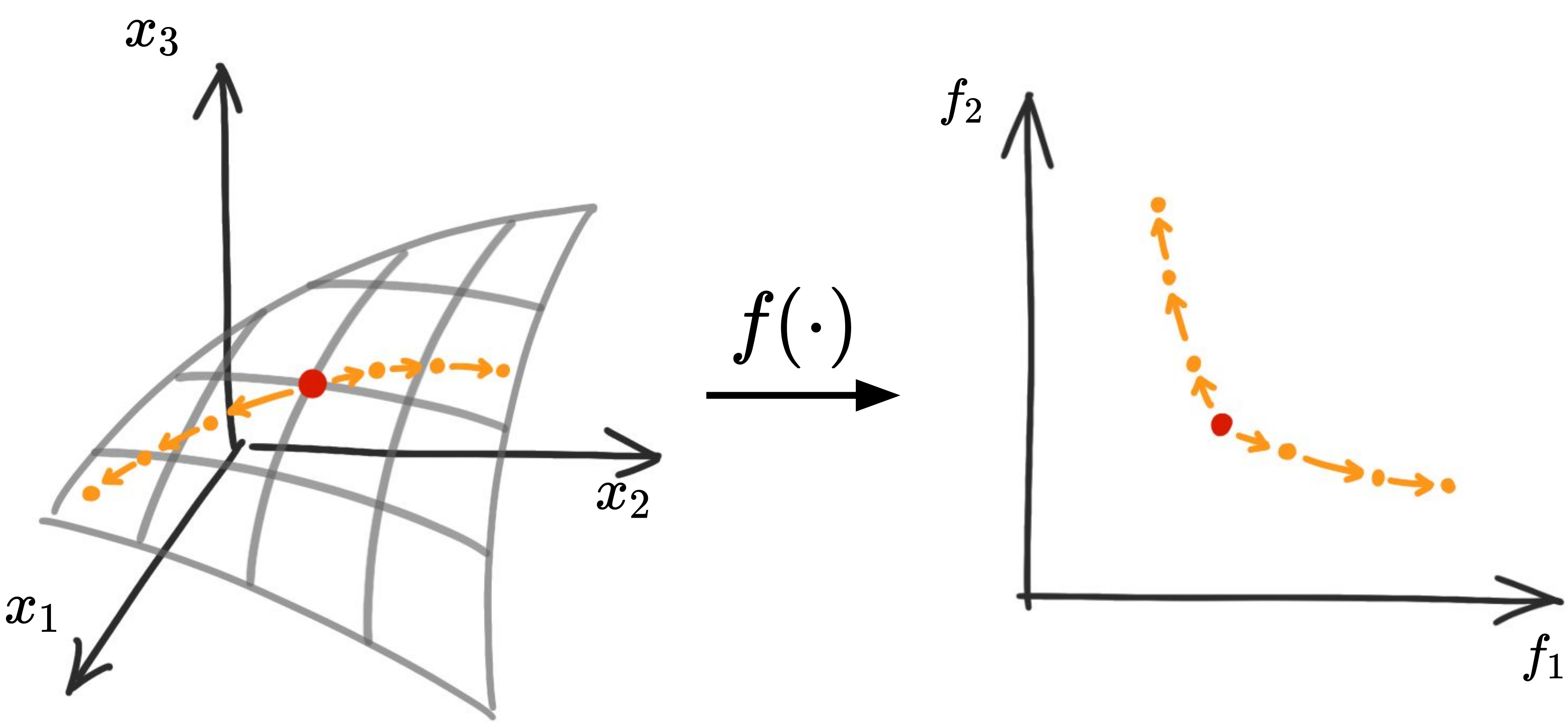
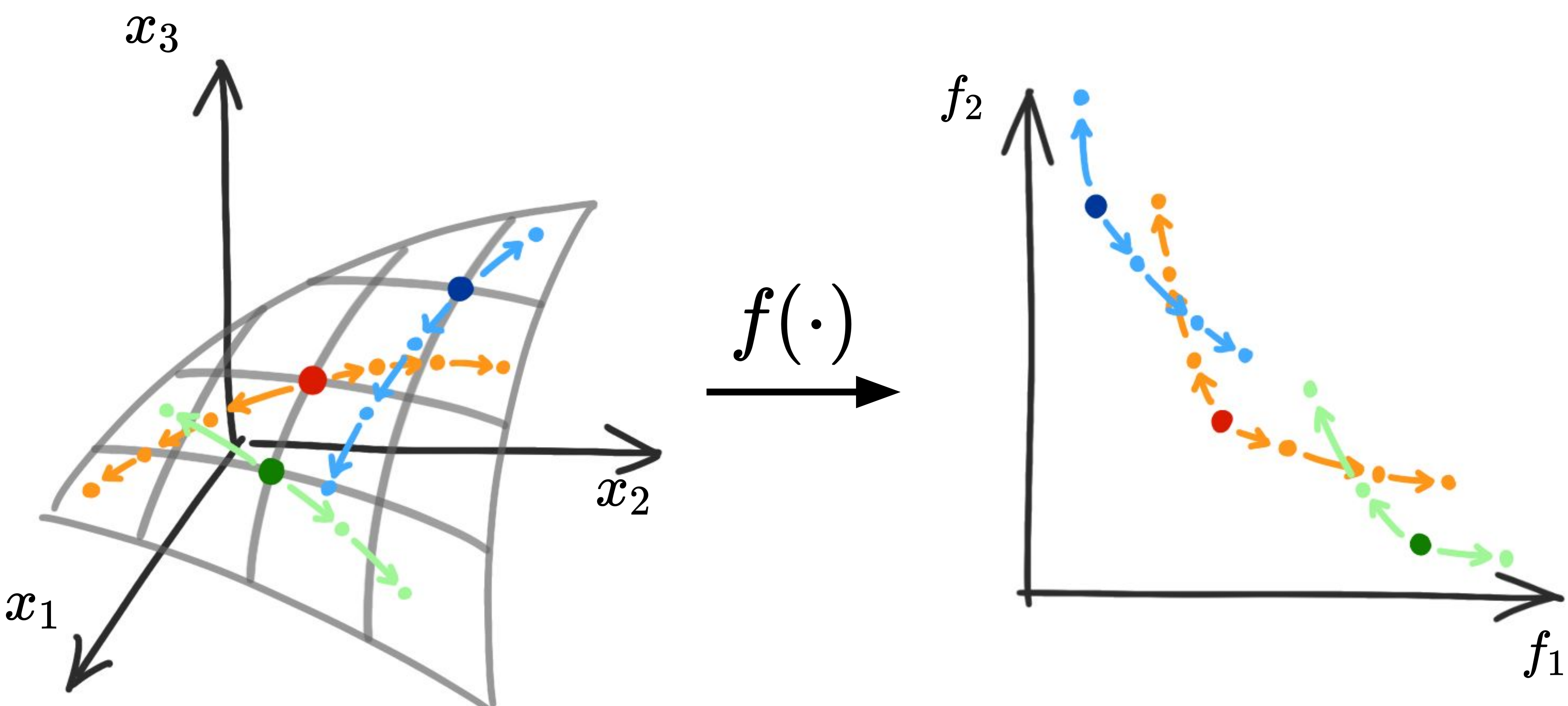


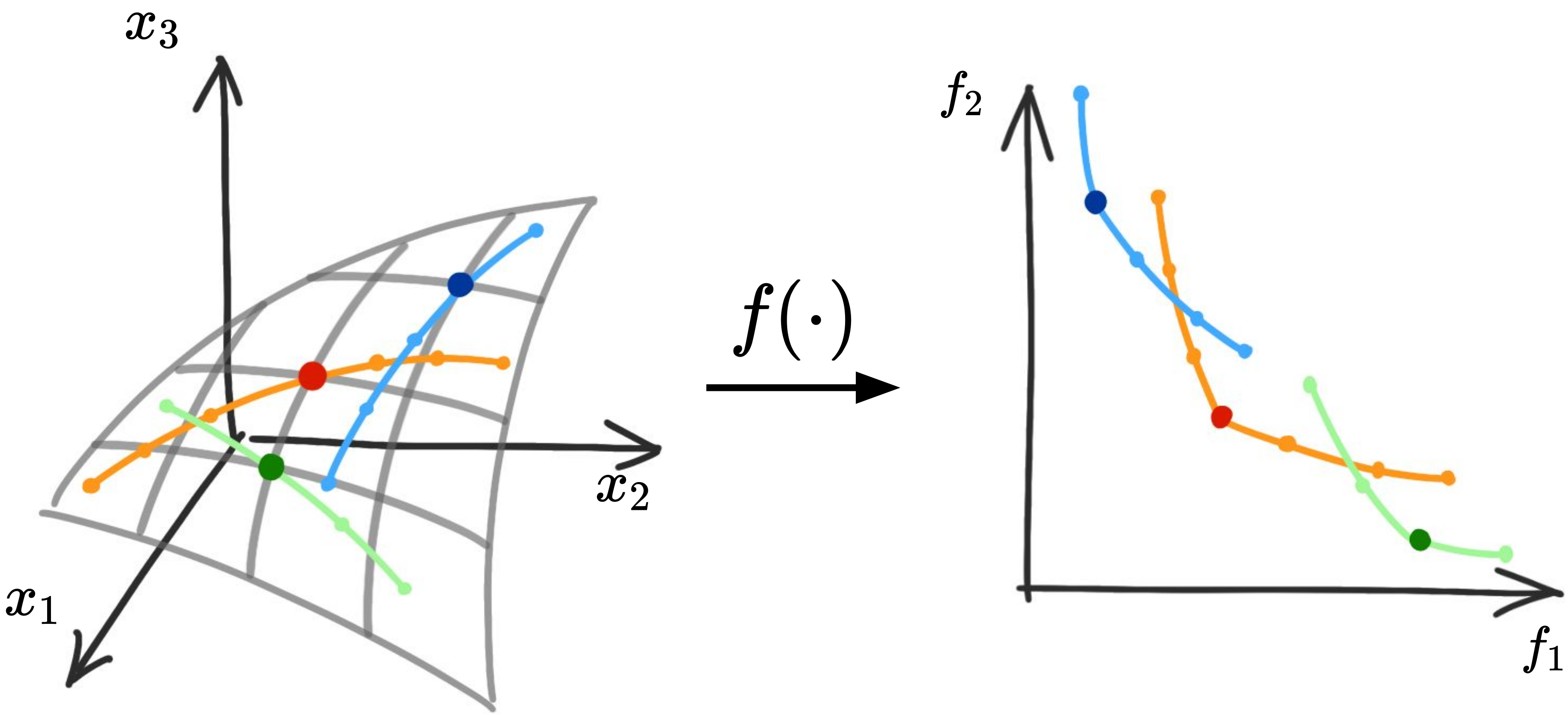
Challenges: Continuous Parameterization

Grow even more solutions from more starting points.



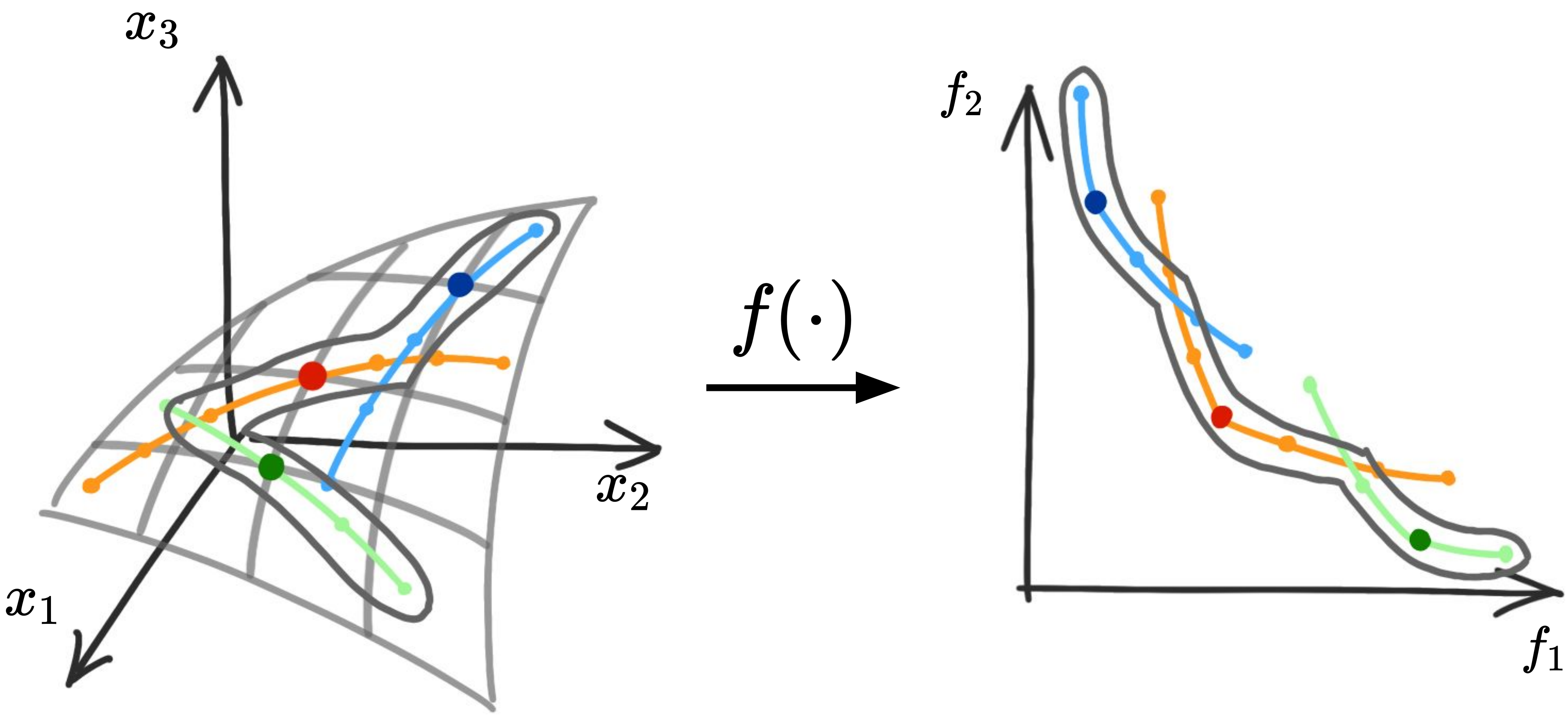
Challenges: Continuous Parameterization

Build continuous parameterization from interpolation.



Challenges: Continuous Parameterization

Filter out others and keep Pareto optimal solutions only.

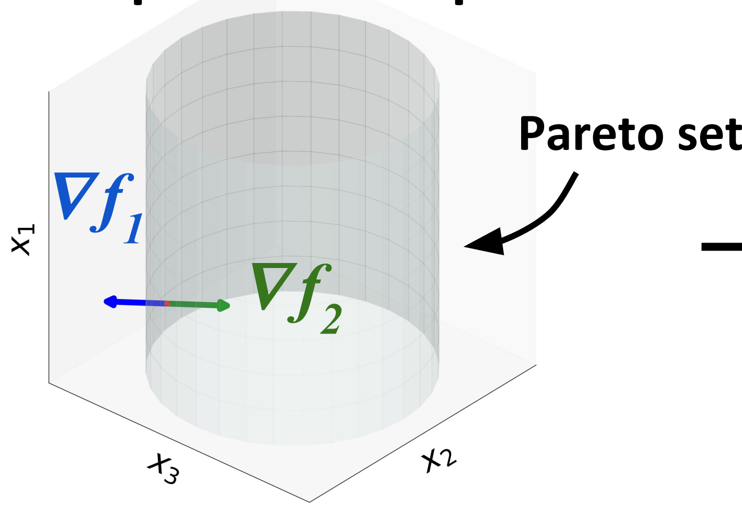


Experiments

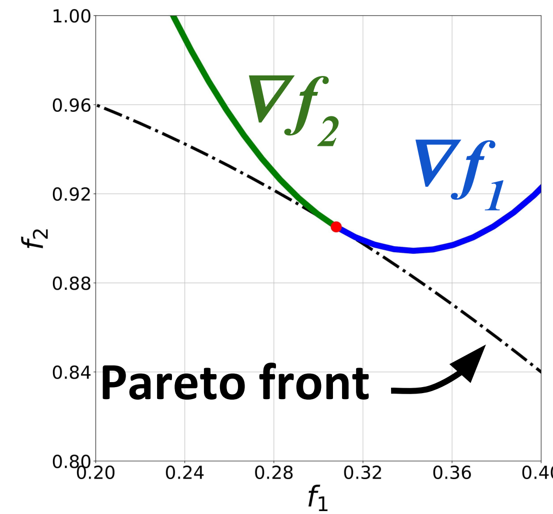
- Synthetic Examples
- Pareto Expansion
- Continuous Parameterization
- Ablation Study

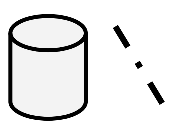
Synthetic Example: ZDT2-Variant

3D parameter space



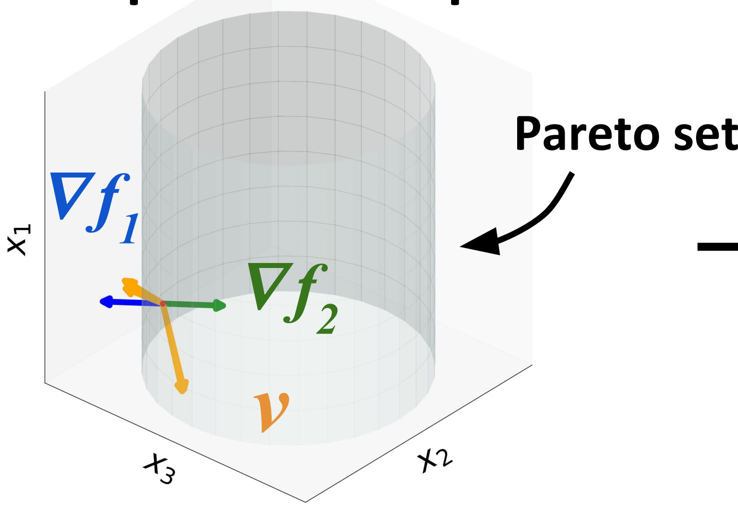
2D performance space



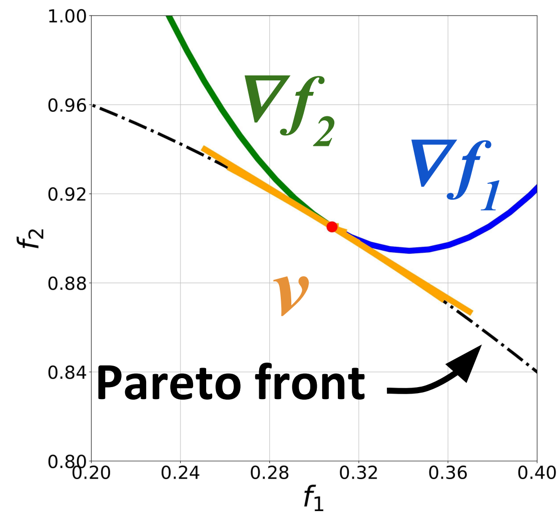
-  = Analytical Pareto set and front
-  = Gradient directions
- Expanding along the gradients deviates from the true Pareto front.

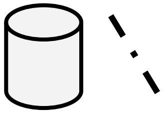
Synthetic Example: ZDT2-Variant

3D parameter space

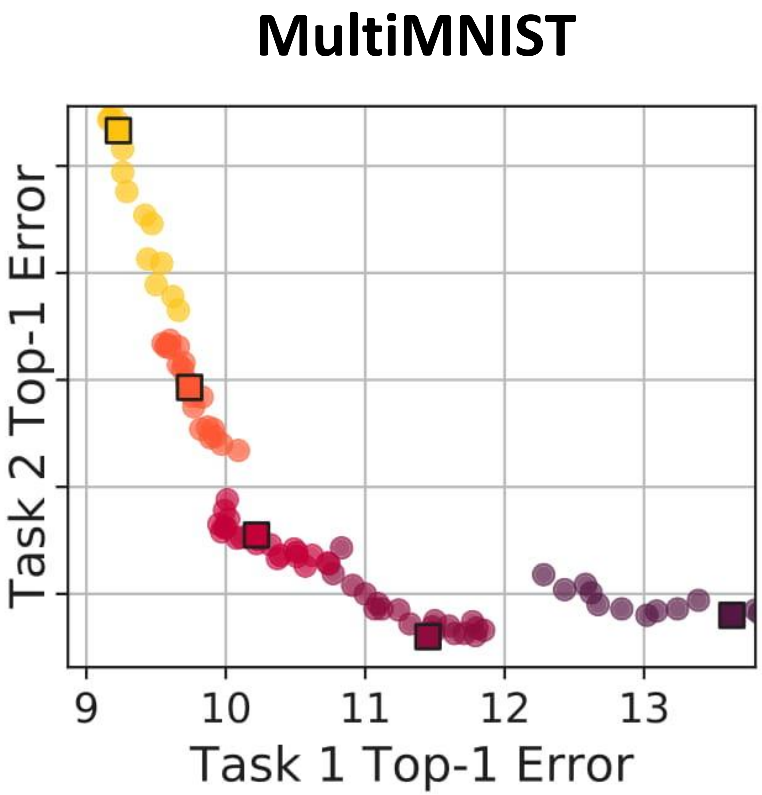


2D performance space



-  = **Analytical Pareto set and front**
- ← = **Our method**
- **Tangent to analytical Pareto set**

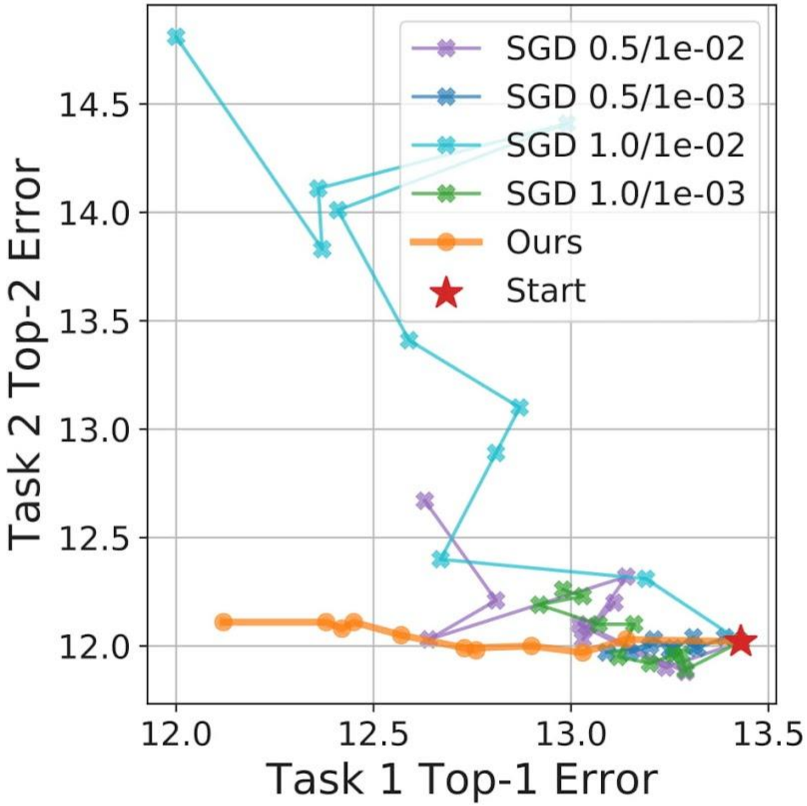
Sufficiency Test



- Color = different start
- Lower left ⇙ = better
- Large coverage

Necessity Test

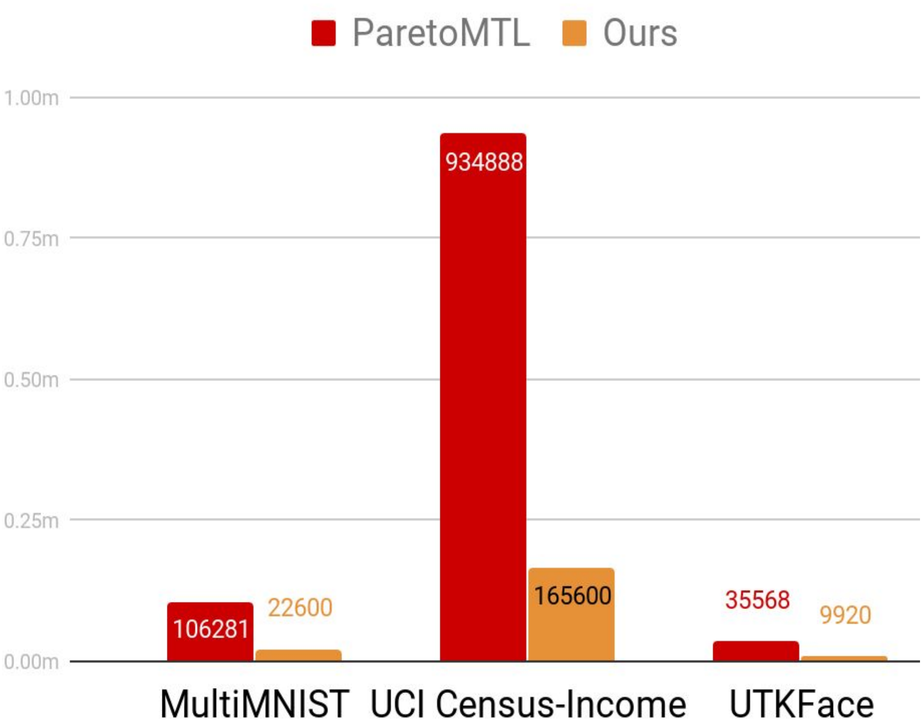
MultiMNIST



- **Expanded from ★**
- **Lower left ⇙ = better**
- **Ours = most effective exploration**

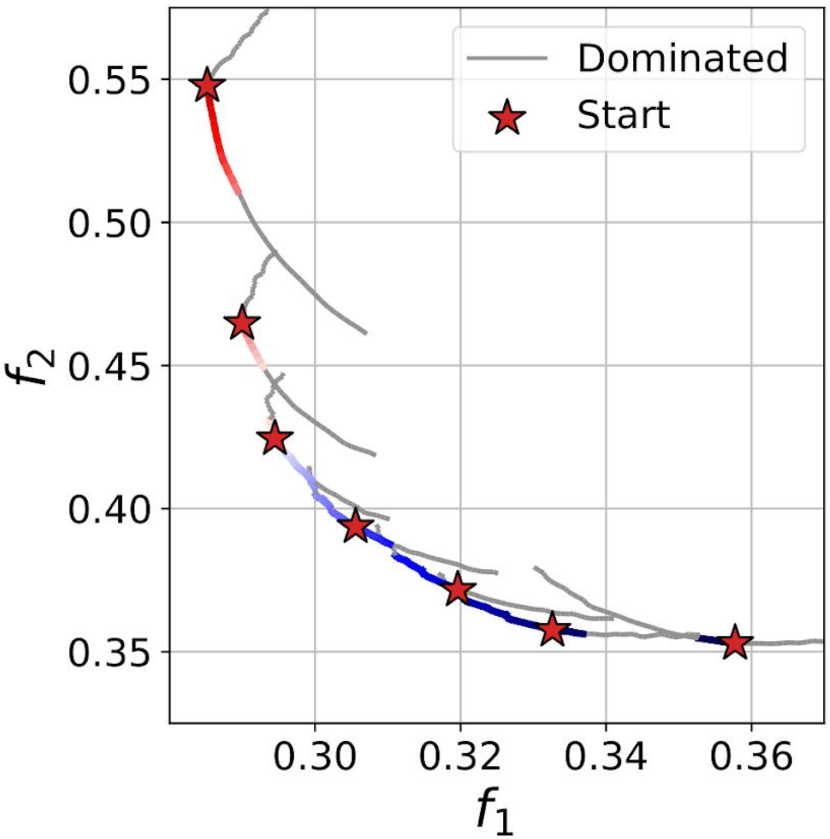
Efficiency Comparison

#Forward/Backward-Propagation



- Our method costs <u>less</u> computation than previous method.

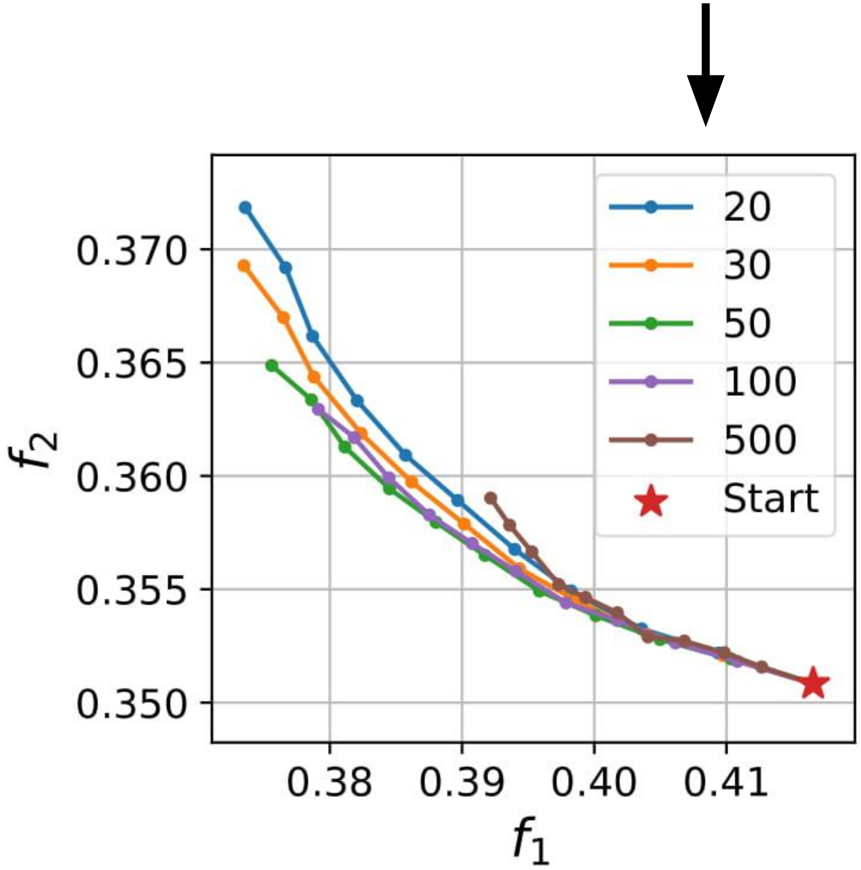
Continuous Parameterization



- Expanded from s
- Red and blue solutions construct the continuous Pareto front
- Gray ones are dominated

Ablation Study: #iteration

#iteration



- Color = #iteration
- Lower left ⇙ = better
- 50 iterations = the best!

Summary

- **Second-order Hessian matrices reveal useful tangent information about Pareto fronts.**

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- **Efficient Hessian-vector product in neural networks unlocks expanding Pareto sets with second-order information.**

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- **Second-order Hessian matrices reveal useful tangent information about Pareto fronts.**
- **Efficient Hessian-vector product in neural networks unlocks expanding Pareto sets with second-order information.**
- **Continuous, first-order accurate Pareto fronts can be obtained by linearly interpolating dense solutions on the tangent plane.**

Thank you!

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Code

https://github.com/mit-gfx/ContinuousParetoMTL