香港中文大學 The Chinese University of Hong Kong
Tencent AI Lab
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TMLR TRUSTWORTHY MACHINE LEARNING AND REASONING

Pareto Invariant Risk Minimization: Towards Mitigating the Optimization Dilemma in OOD Generalization

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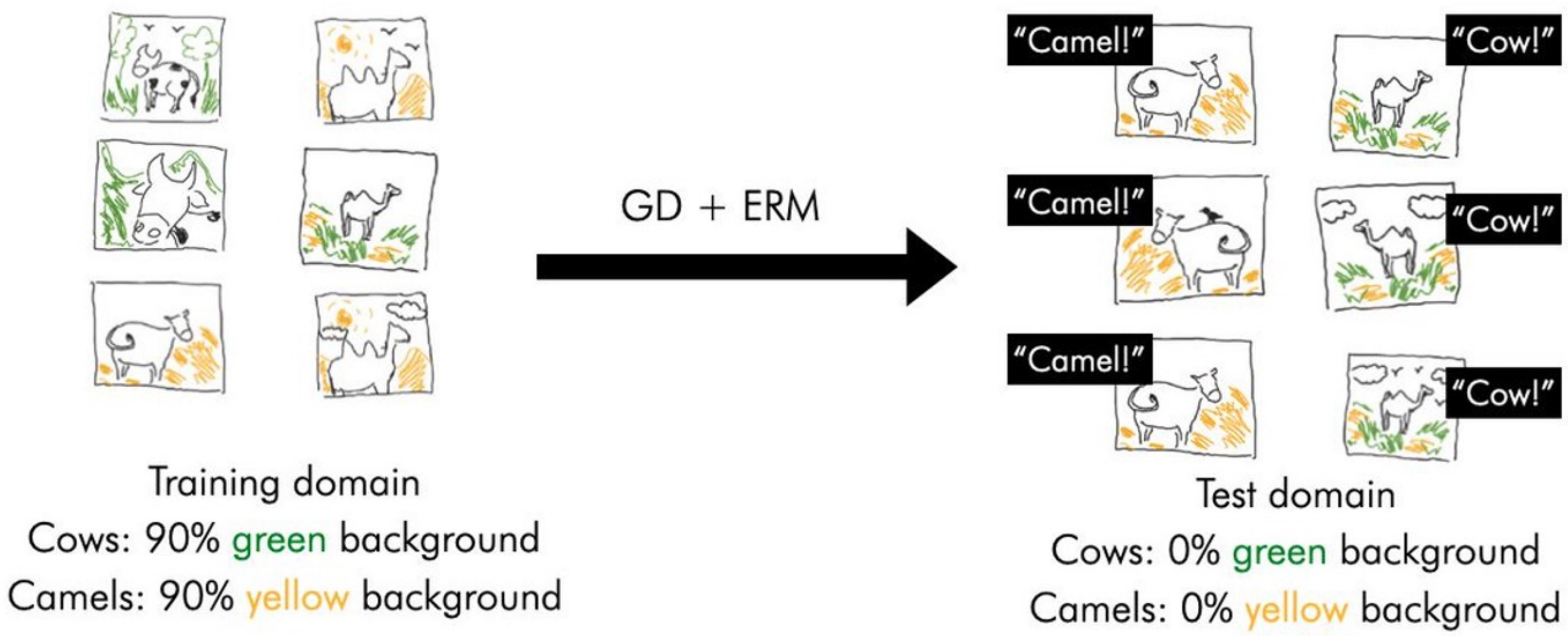
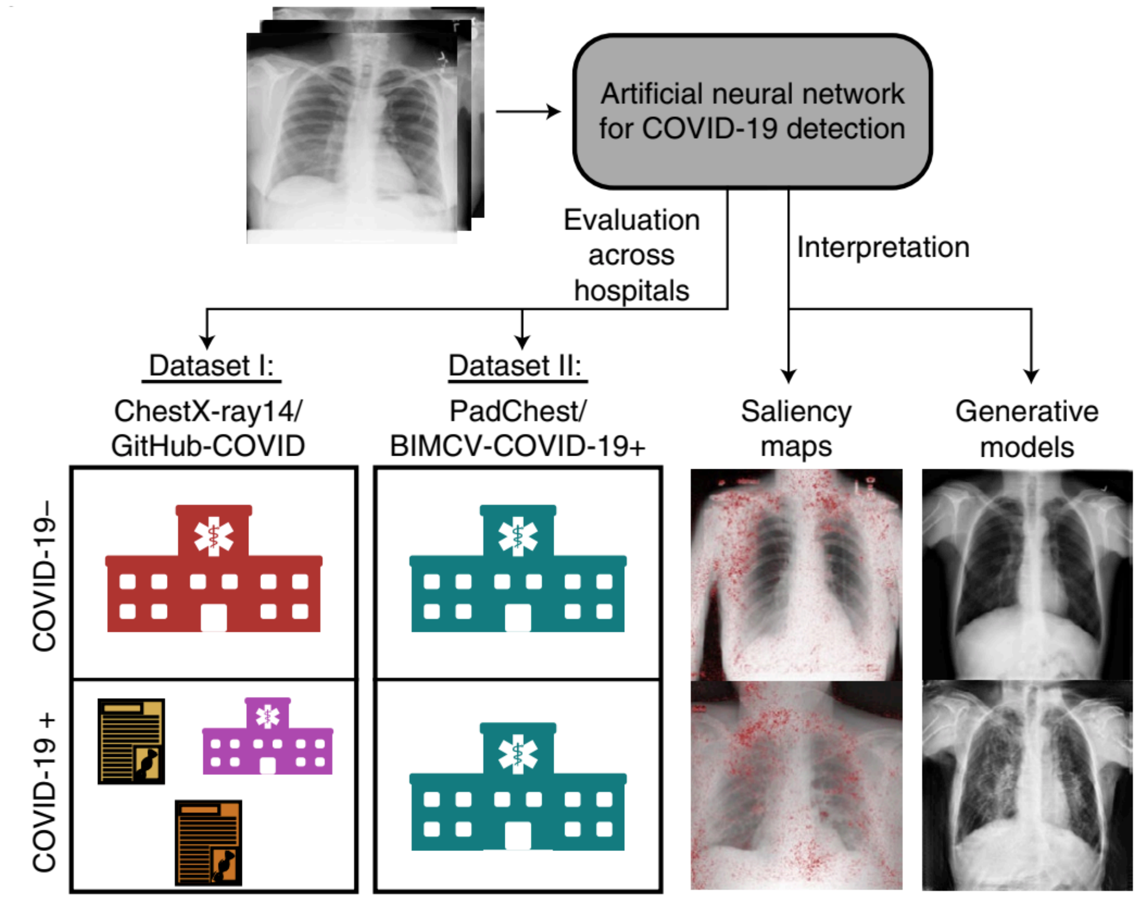
with Kaiwen Zhou, Yatao Bian, Binghui Xie,
Bingzhe Wu, Peilin Zhao, Bo Han, James Cheng and others.

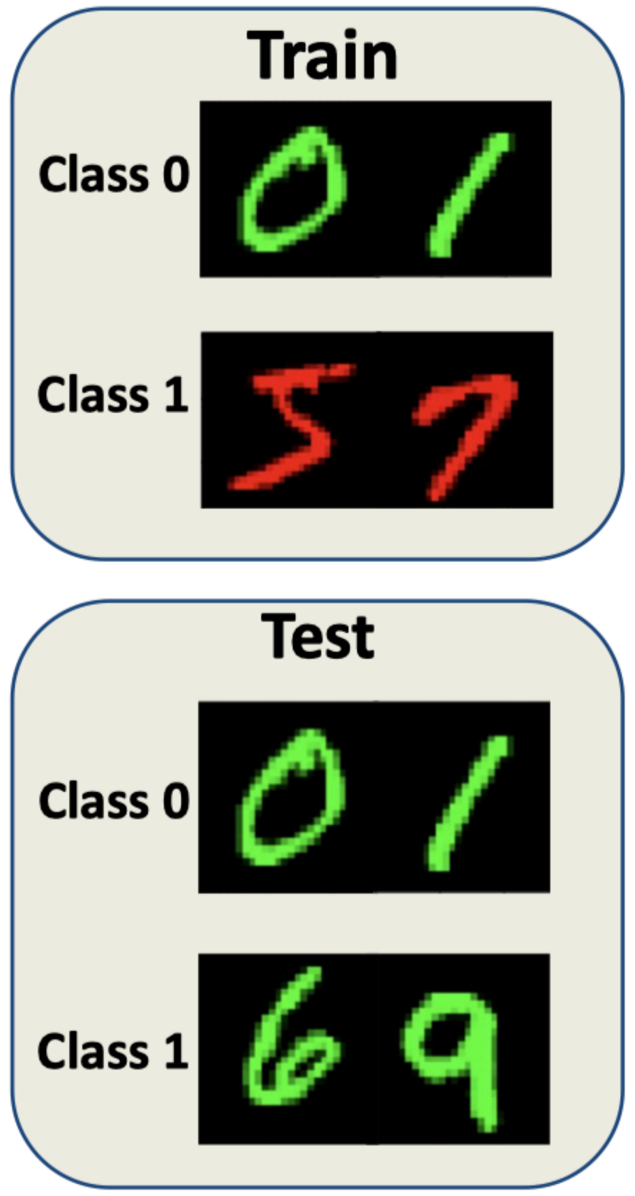
Out-of-Distribution generalization





b

	Dataset I			Dataset II		
	Combined	Chest-X-ray14	GitHub-COVID	Combined	PadChest	BIMCV-COVID-19+
No. radiographs	112,528	112,120	408	97,866	96,270	1,596
No. patients	31,067	30,805	262	64,954	63,939	1,105
% COVID-19+	0.2	0	76.5	1.6	0	100
% AP images	39.9	40	26	5.6	4.7	58.1



(Beery et al., 2018; Arjovsky et al., 2019; DeGrave et al. 2021; Ahuja et al., 2021; Zhang et al., 2022)

Models trained with Empirical Risk Minimization (ERM) are often:

- prone to **spurious correlations**

- can hardly generalize to **OOD** data

Previous works focus on OOD objectives

Previous works mostly focus on developing better ***optimization objectives***:

$$\min_f L_{\text{ERM}} + \lambda \cdot \boxed{\widehat{L}_{\text{OOD}}}$$

Regularization via some OOD objective

(Arjovsky et al., 2019; Krueger et al., 2021; Rame et al., 2021; Pezeshki et al., 2021; Ahuja et al., 2021; Zhang et al., 2022)

The Optimization Dilemma in OOD Generalization

Previous works mostly focus on developing better ***optimization objectives***:

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Regularization via some ***relaxed*** OOD objective

(Arjovsky et al., 2019; Kamath et al., 2021)

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Regularization via some ***relaxed*** OOD objective

$$\min_{f=w\circ\varphi} \sum_{e\in\mathscr{E}_{\text{tr}}} \mathscr{L}_e(w\circ\varphi),$$
$$\text{s.t. } w \in \arg\min_{\bar{w}} \mathscr{L}_e(\bar{w}\circ\varphi),\ \forall e\in\mathscr{E}_{\text{tr}}$$

$$\min_{\varphi} \sum_{e\in\mathscr{E}_{\text{tr}}} \mathscr{L}_e(\varphi),$$
$$\text{s.t. } \nabla_{w|w=1}\mathscr{L}_e(w\cdot\varphi) = 0,\ \forall e\in\mathscr{E}_{\text{tr}}$$

$$\min_{\varphi} \sum_{e\in\mathscr{E}_{\text{tr}}} \mathscr{L}_e(\varphi) + \lambda\|\nabla_{w|w=1}\mathscr{L}_e(w\cdot\varphi)\|^2$$

Linearized IRM with $w \in \mathbb{R}^d$

Soften the constraints

IRM 😋

$\text{IRM}_{\mathcal{S}}$ 😢

IRMv1 😢 😢

(Arjovsky et al., 2019; Kamath et al., 2021)

The Optimization Dilemma in OOD Generalization

🥲 The practical variants of IRM can have very different behaviors from the original IRM.

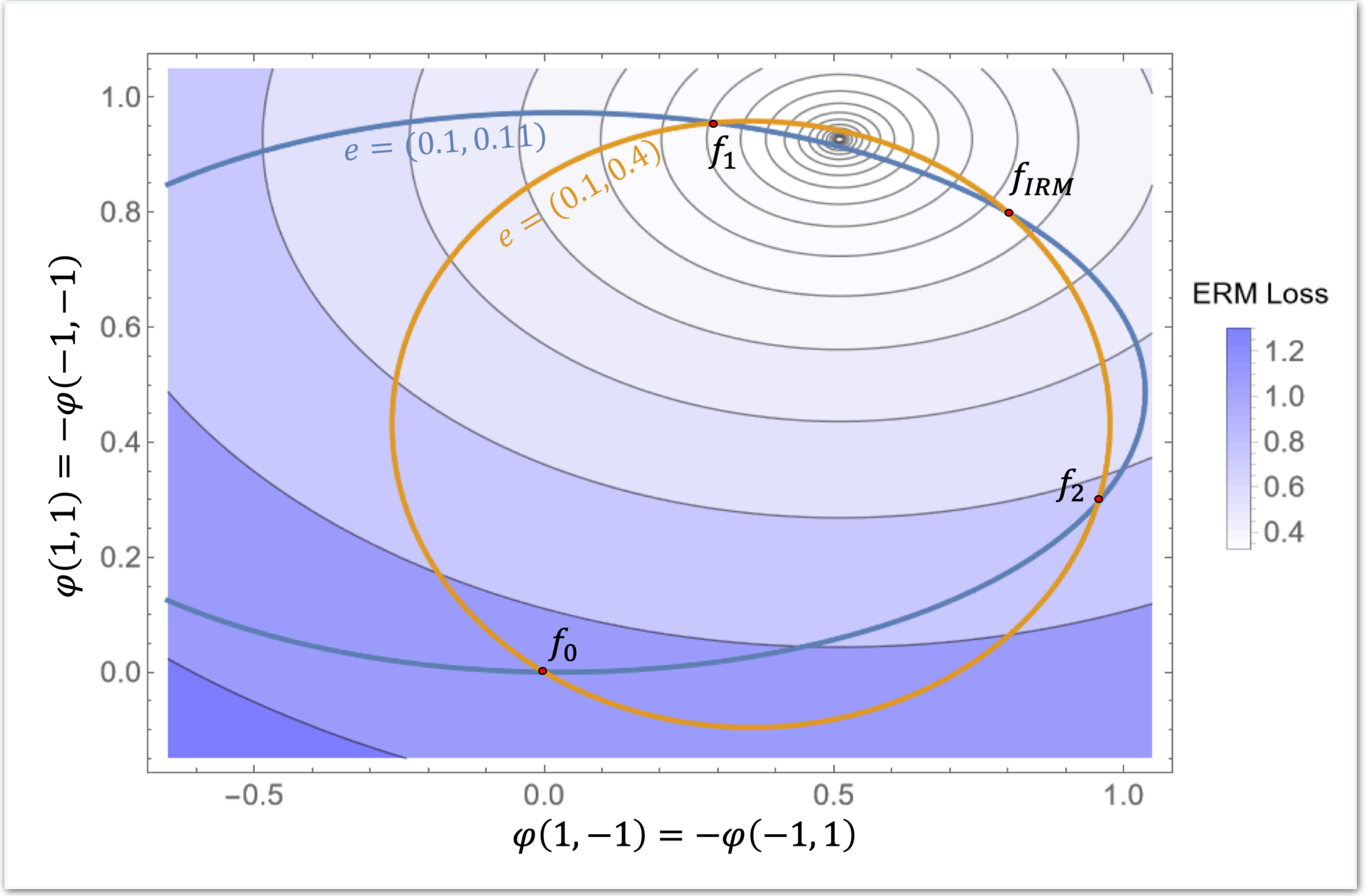

Illustration of IRMv1 failures

The ellipsoids are the solutions satisfying the **invariant constraints** in $\mathrm{IRM}_{\mathcal{S}}$

$$\nabla_{w|w=1}\mathcal{L}_e(w \cdot \varphi) = 0, \forall e \in \mathcal{E}_{\mathrm{tr}}$$

(Arjovsky et al., 2019; Kamath et al., 2021)

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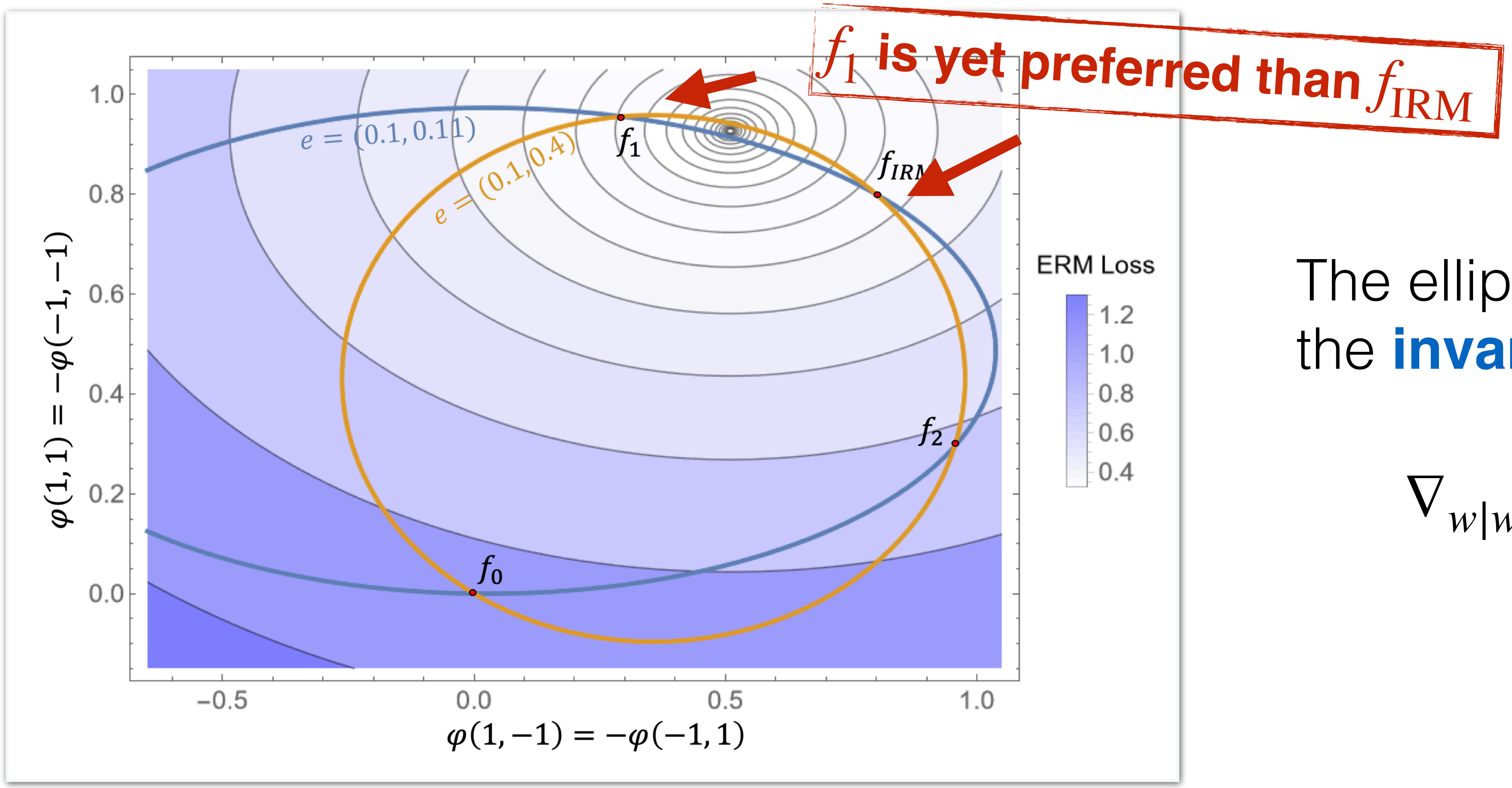

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(Arjovsky et al., 2019; Kamath et al., 2021)

The Optimization Dilemma in OOD Generalization

Previous works mostly focus on developing better ***optimization objectives***:

$$\min_f L_{\mathrm{ERM}} + \lambda \cdot \widehat{L}_{\mathrm{OOD}}$$

λ is ***hard to tune***

(Arjovsky et al., 2019; Krueger et al., 2021; Rame et al., 2021; Pezeshki et al., 2021; Ahuja et al., 2021; Zhang et al., 2022)

The Optimization Dilemma in OOD Generalization

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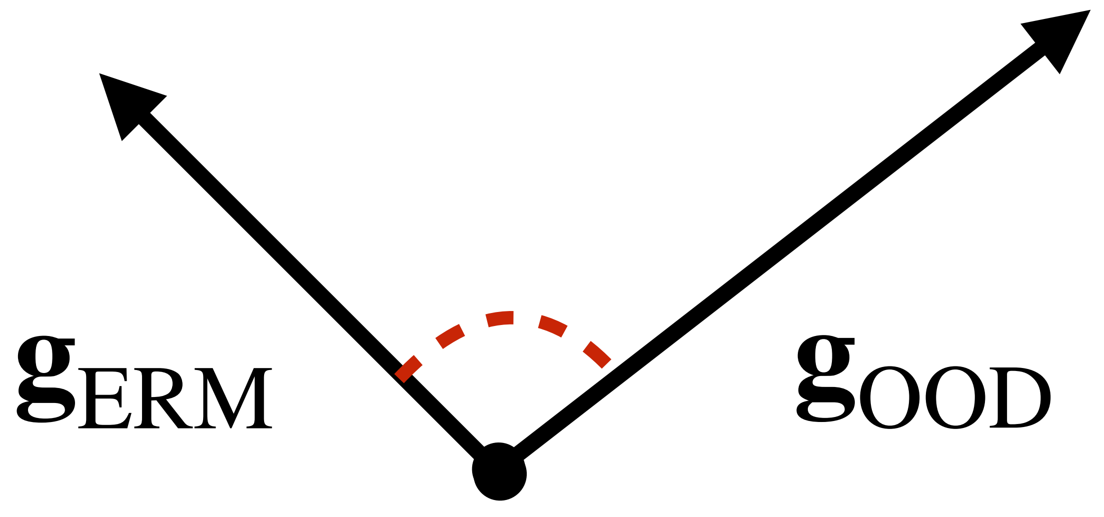
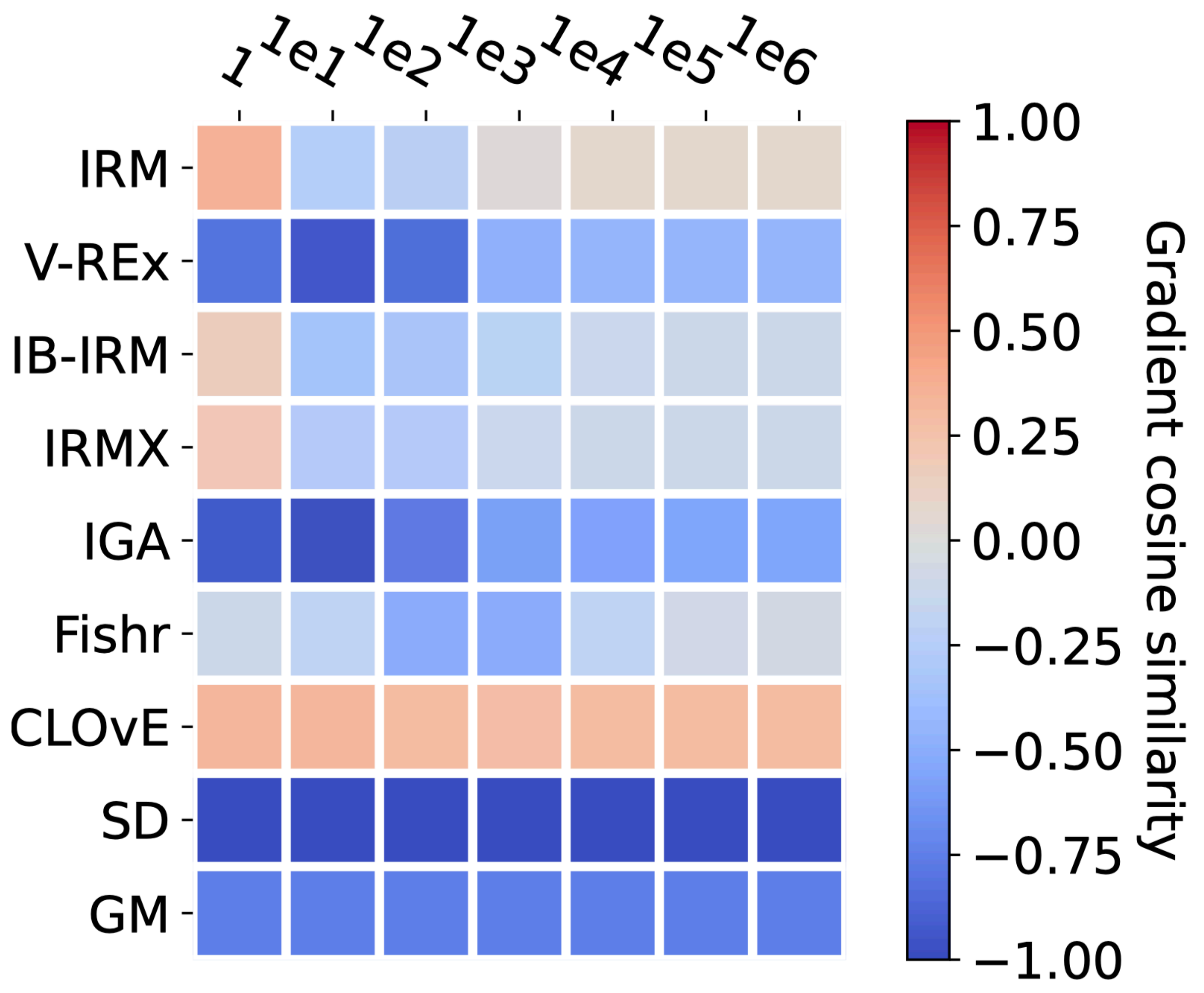
Gradient Conflicts generically exist between ERM and OOD objectives:





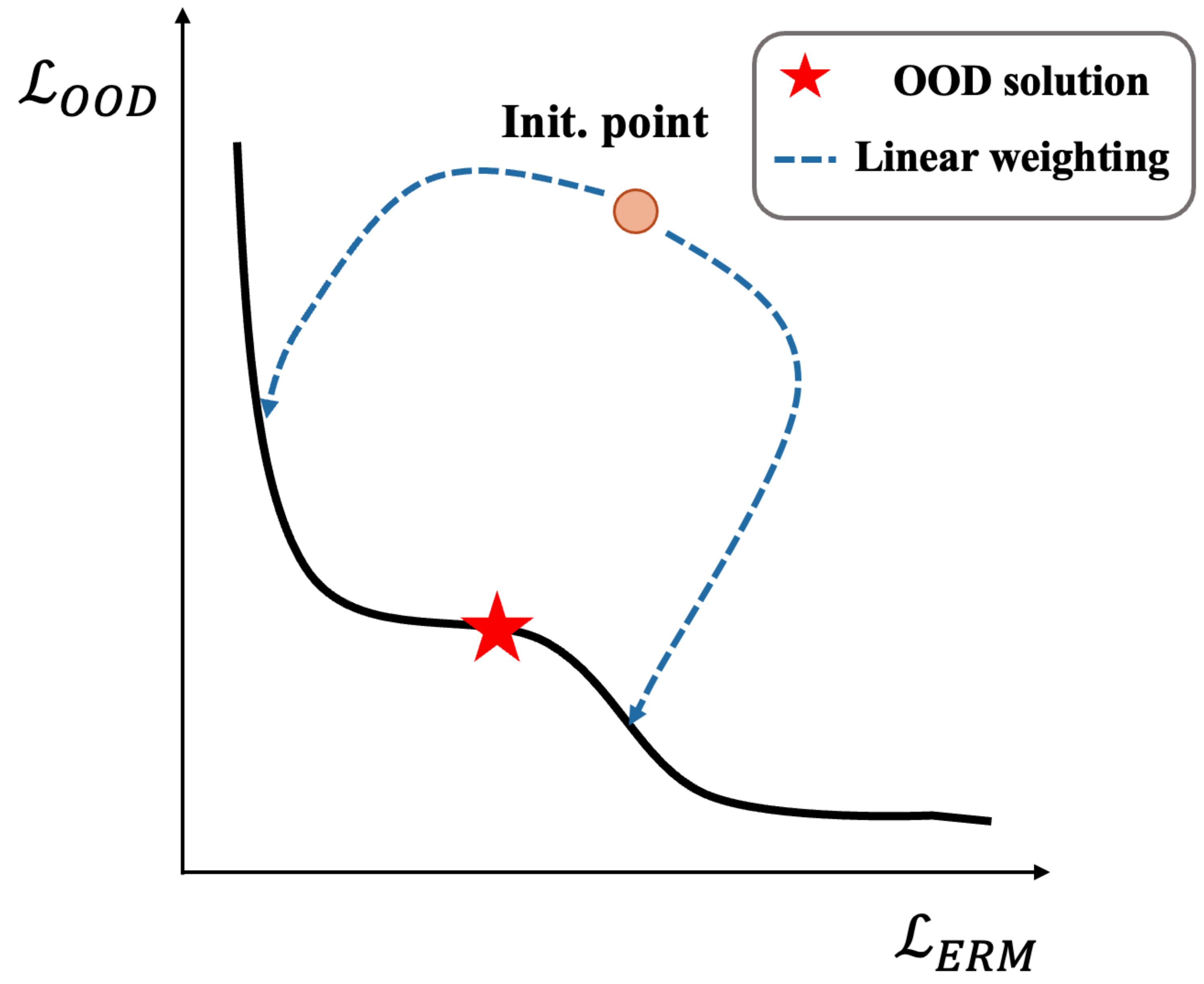
(Arjovsky et al., 2019; Krueger et al., 2021; Rame et al., 2021; Pezeshki et al., 2021; Ahuja et al., 2021; Zhang et al., 2022)

The Optimization Dilemma in OOD Generalization

The typically used linear weighting scheme cannot reach ***non-convex part of pareto front solutions***

$$\boxed{\min_f L_{\mathrm{ERM}} + \lambda \cdot \widehat{L}_{\mathrm{OOD}}}$$

The linear weight scheme

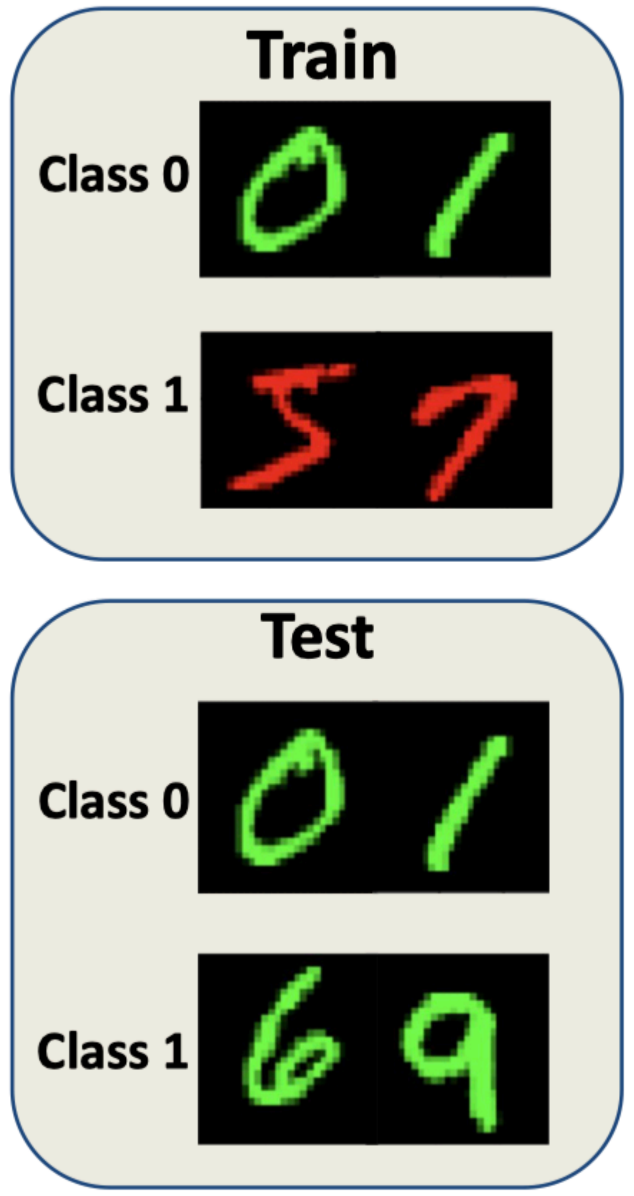


(Boyd & Vandenberghe, 2014)

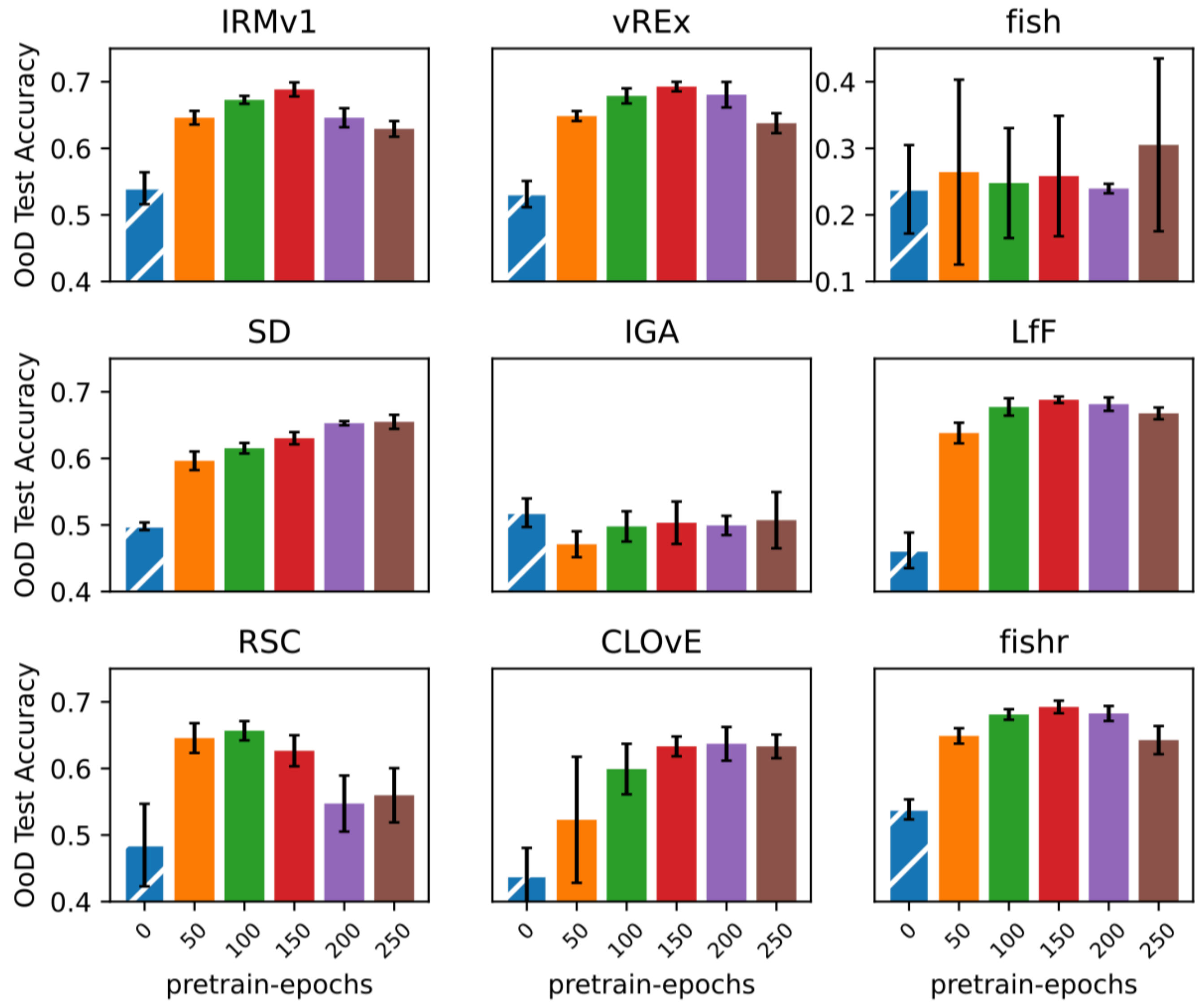
The Optimization Dilemma in OOD Generalization

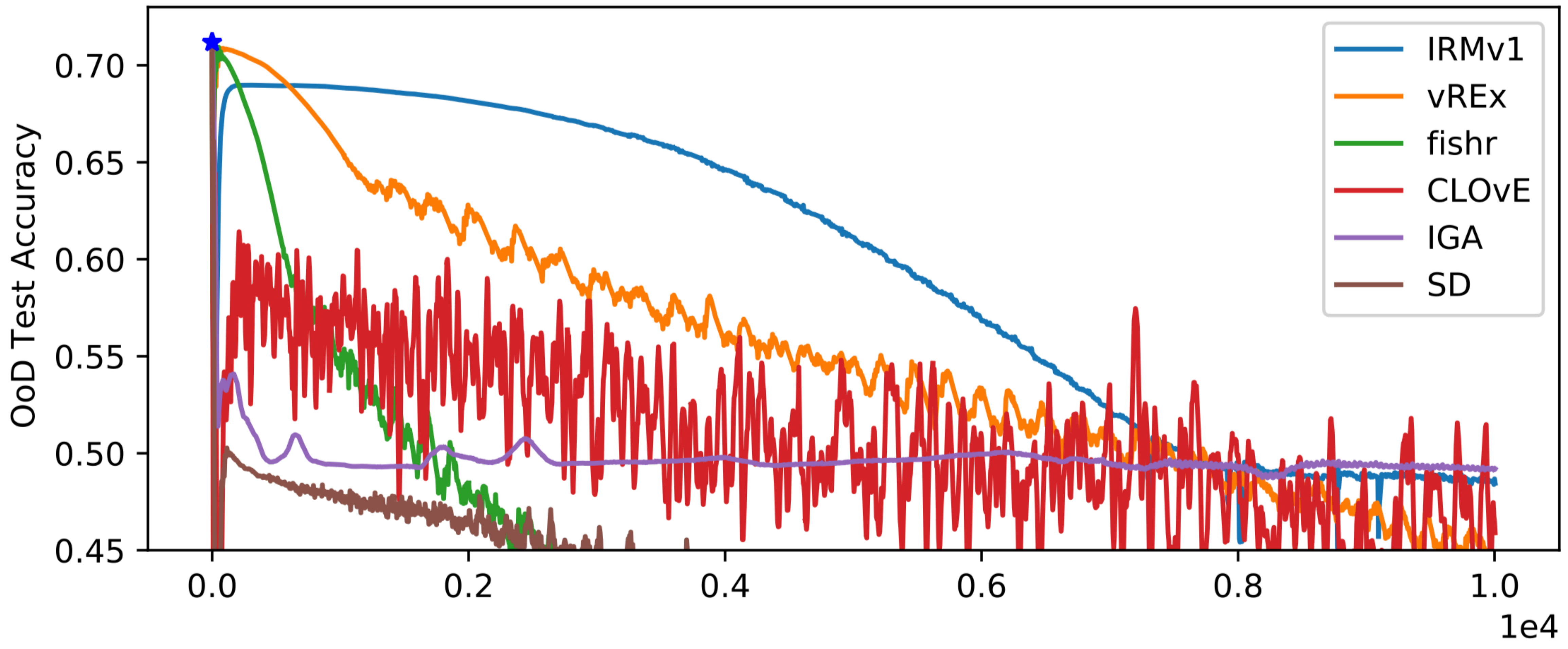
Even the desired solution is reachable, the scheme requires ***exhaustive hyperparemter tuning***:

$$\min_f L_{\text{ERM}} + \lambda \cdot \widehat{L}_{\text{OOD}}$$



λ is ***too strong*** to learn the correlation; λ is ***too weak*** to keep the invariance





(Arjovsky et al., 2019; Krueger et al., 2021; Rame et al., 2021; Pezeshki et al., 2021; Ahuja et al., 2021; Zhang et al., 2022)

The Optimization Dilemma in OOD Generalization

The usual optimization formula of OOD objectives in practice:

$$\min_f L_{\text{ERM}} + \boxed{\lambda} \cdot \boxed{\widehat{L}_{\text{OOD}}}$$

λ is ***hard to tune*** Regularization via some ***relaxed*** OOD objective

- $\widehat{L}_{\text{OOD}}$ usually has ***a large gap*** from the original one;
- λ is ***hard to tune***, i.e.,
  - Not all potentially optimal solutions are reachable;
  - Even reachable, it still requires exhaustive tuning efforts to find a proper λ;

(Arjovsky et al., 2019; Krueger et al., 2021; Rame et al., 2021; Pezeshki et al., 2021; Ahuja et al., 2021; Zhang et al., 2022)

As the traditional optimization scheme fails

How to obtain a desired OOD solution under the ERM and OOD conflicts?

From a Multi-Objective Optimization perspective…

The optimization of IRM essentially handles the ***trade-off*** between

$$\min_f \boxed{L_{\text{ERM}}} + \lambda \cdot \boxed{\widehat{L}_{\text{OOD}}}$$

Capturing the statistical correlations

Enforcing the invariance of learned correlations

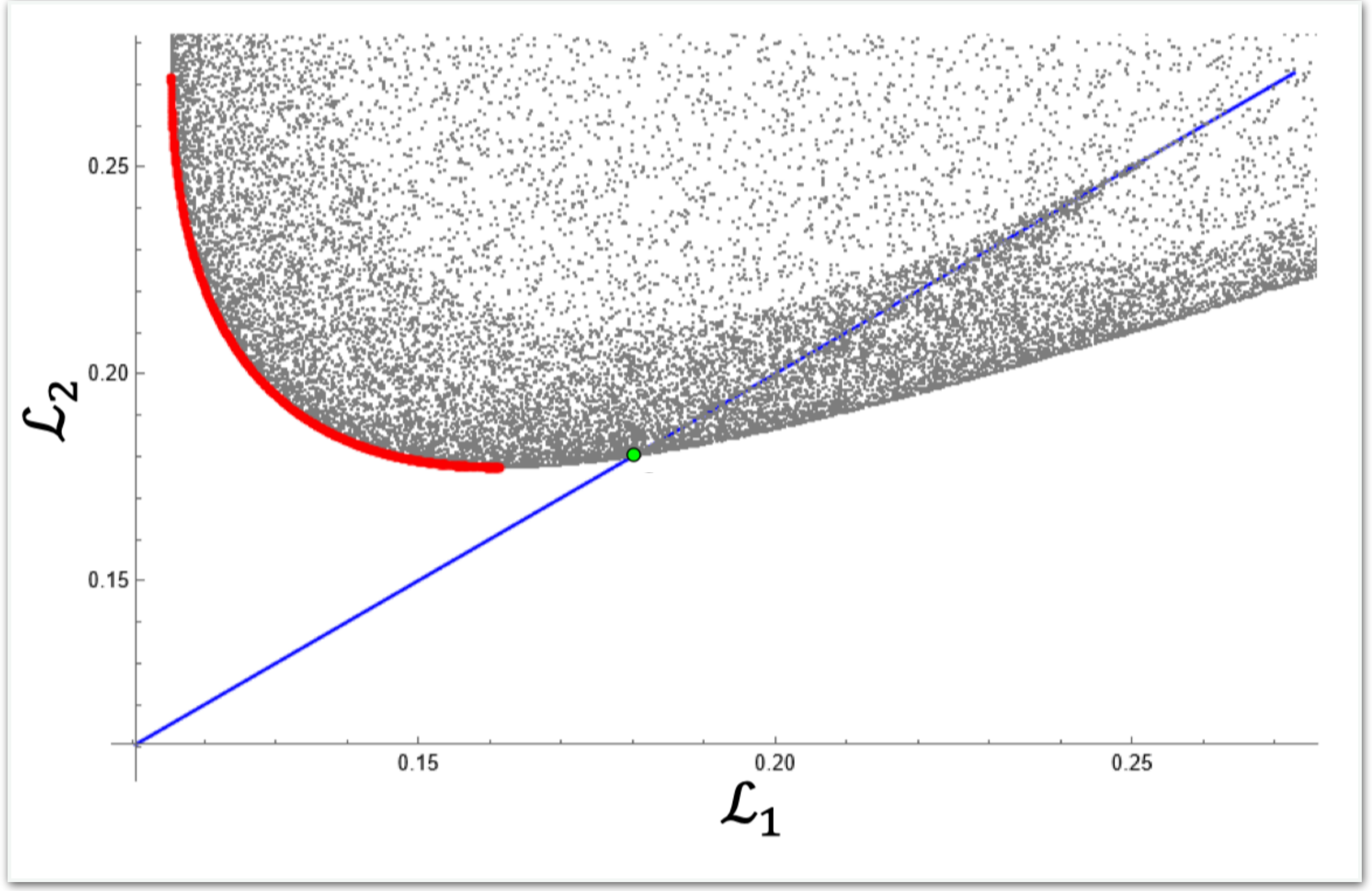
Oh, it's a Multi-Objective Optimization (MOO)!

$$\min_f \{L_{\text{ERM}}, \quad \widehat{L}_{\text{OOD}}\}^T$$

From a Multi-Objective Optimization perspective…

Assume we have the Multi-Objective Optimization (MOO) problem with 2 objectives:

$$\min_{f=w\cdot\varphi} \{L_1, L_2\}^T$$



Simulated Pareto front

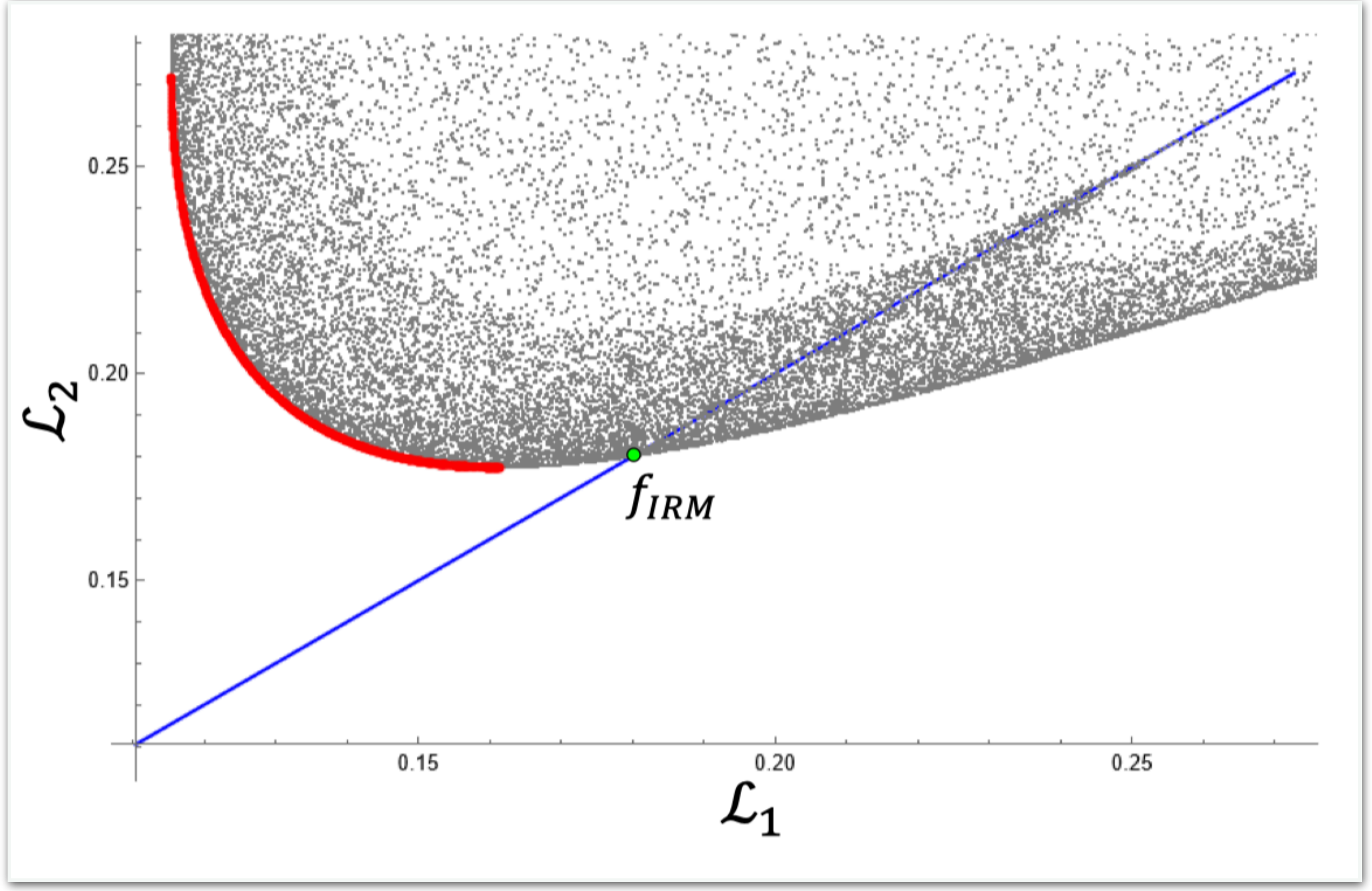
- A solution f (with $\{L_1, L_2\}^T$) **dominates** $\bar{f}$ (with $\{\bar{L}_1, \bar{L}_2\}^T$) if both $L_1 \leq \bar{L}_1$ and $L_2 \leq \bar{L}_2$;
- **Pareto optimal solutions** are the set of solutions dominated by none;
- Their images form the **Pareto front**;

(Kaisa, 1999)

From a Multi-Objective Optimization perspective…

Assume we have 2 training environments, a natural MOO formulation of IRMv1 is:

$$\min_{f=w\cdot\varphi} \{L_1, L_2, L_{\mathrm{IRM}}\}^T$$



Simulated Pareto front

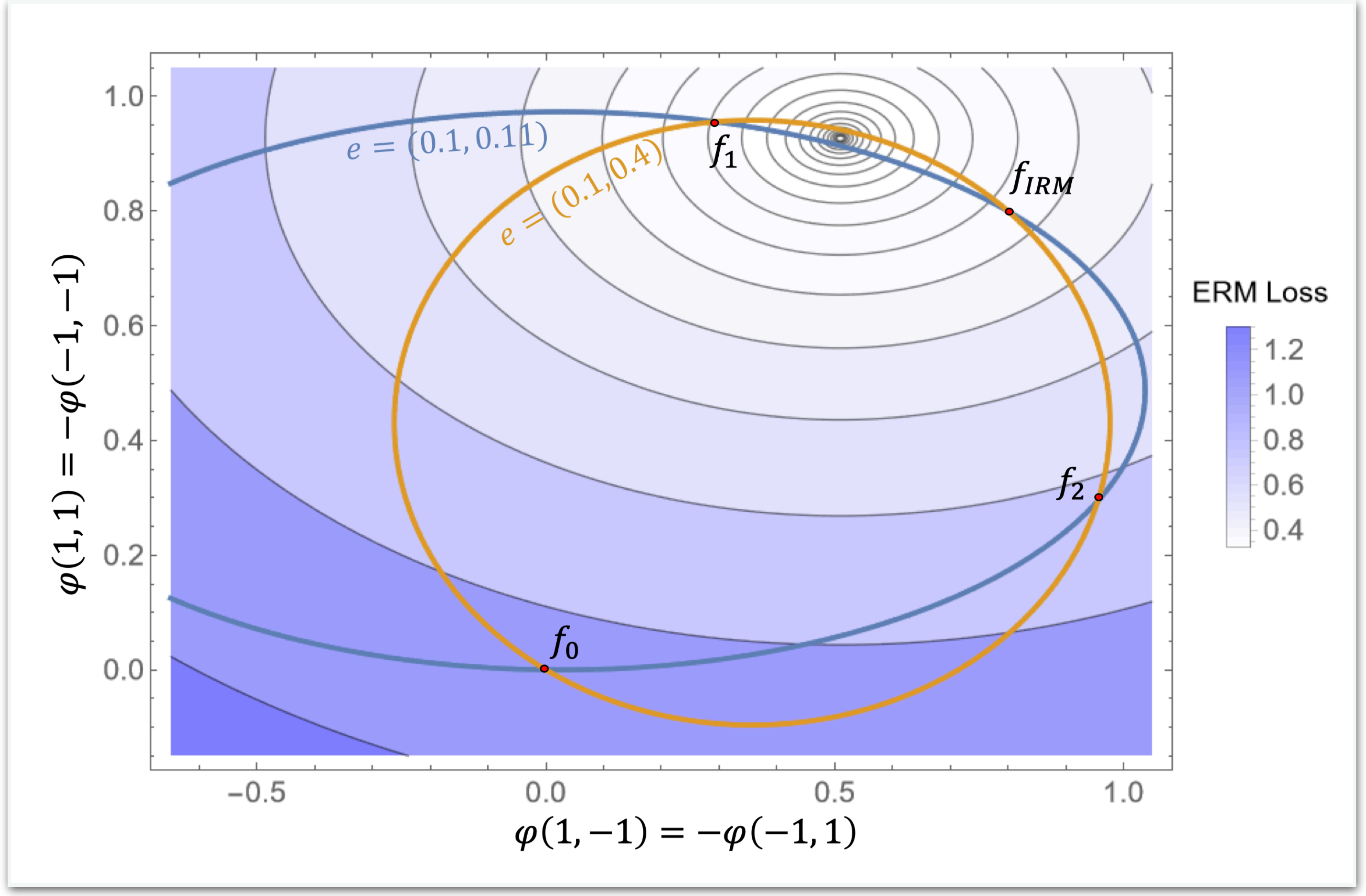
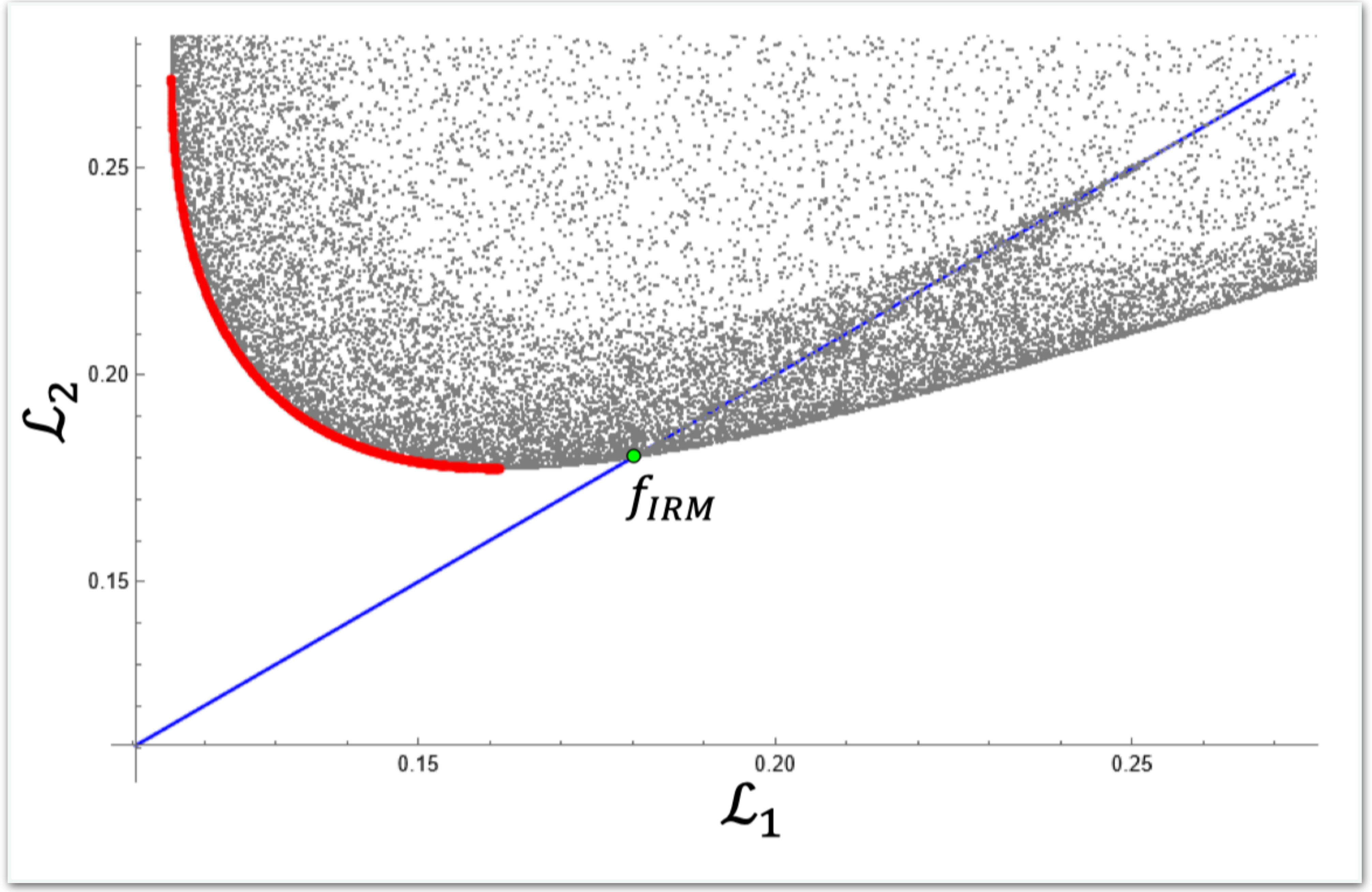


Illustration of IRMv1 failures

From a Multi-Objective Optimization perspective…

The failures of practical IRM variants is because of using **bad objectives**!

$$\min_{f=w\cdot\varphi} \{L_1, L_2, L_{\mathrm{IRM}}\}^T$$



Simulated Pareto front

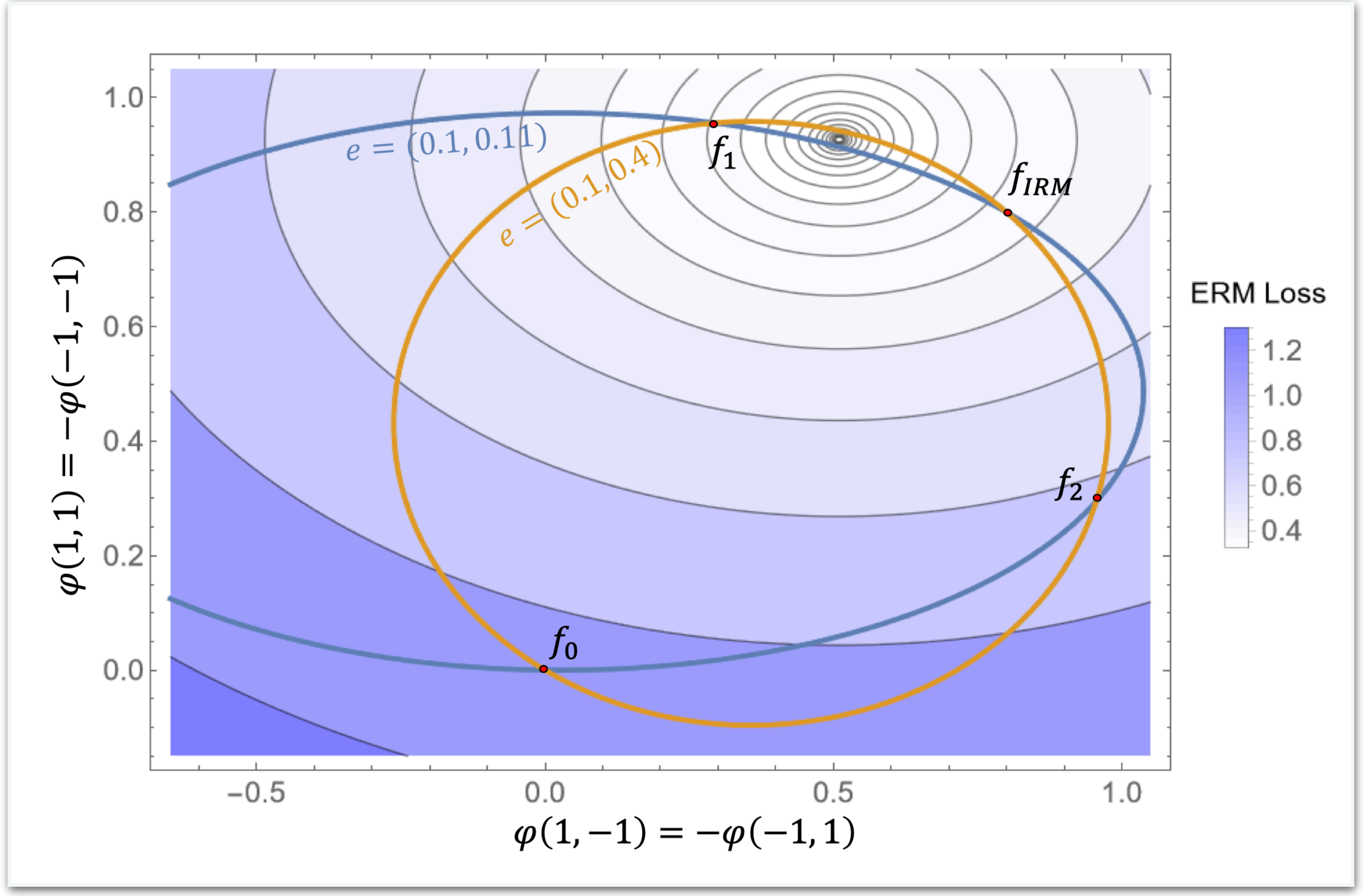
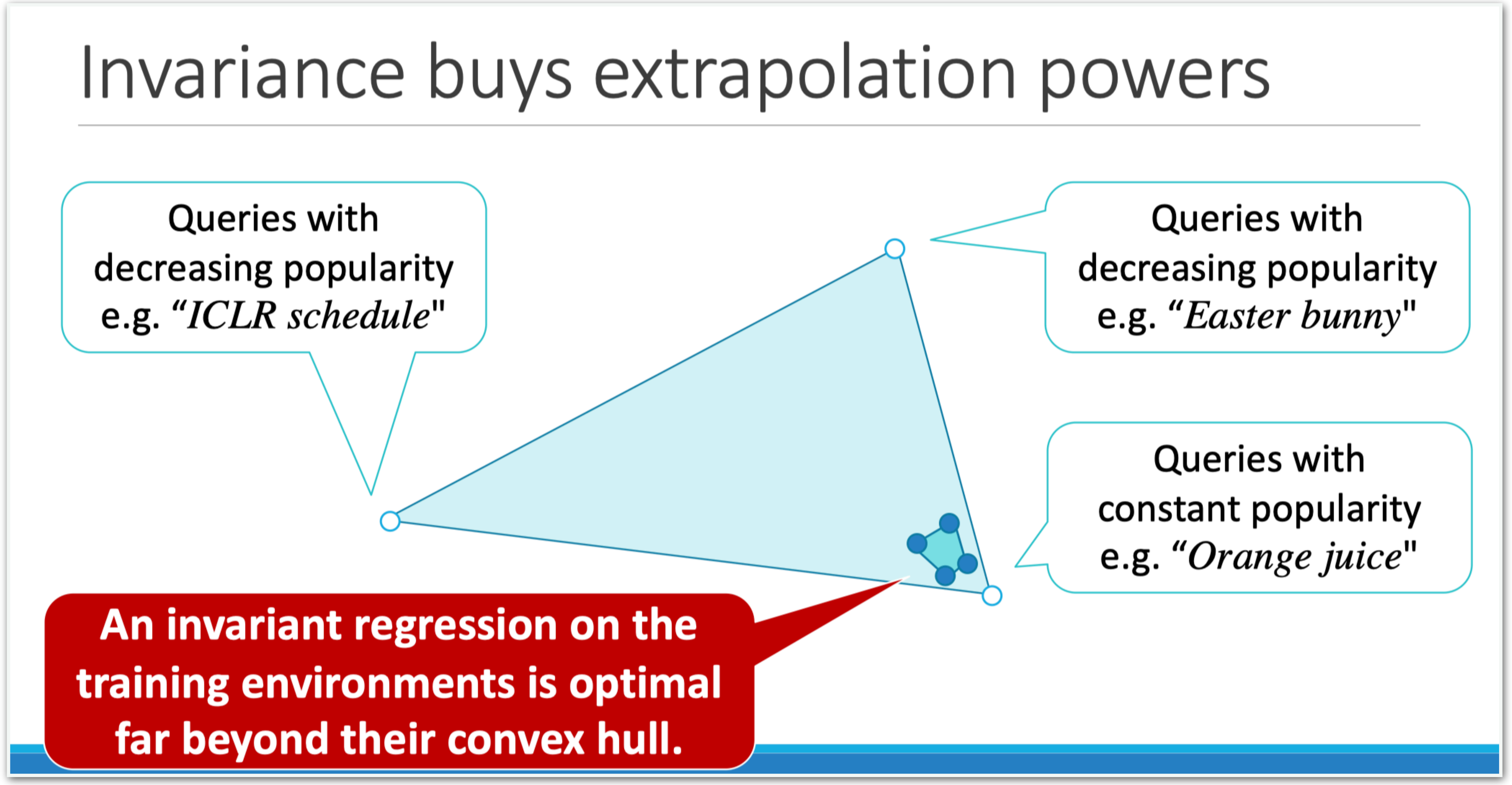


Illustration of IRMv1 failures

Robustify MOO objectives

IRM can extrapolate **stationary points** of **negative** combinations of training environments:

$$\{\sum_{e\in\mathscr{E}_{\mathrm{tr}}} \lambda_e \mathscr{D}_e \mid \sum_{e\in\mathscr{E}_{\mathrm{tr}}} \lambda_e = 1, \lambda_e \geq 0, \forall e\} \Rightarrow \{\sum_{e\in\mathscr{E}_{\mathrm{tr}}} \lambda_e \mathscr{D}_e \mid \sum_{e\in\mathscr{E}_{\mathrm{tr}}} \lambda_e = 1, \lambda_e \leq 0, \forall e\}$$

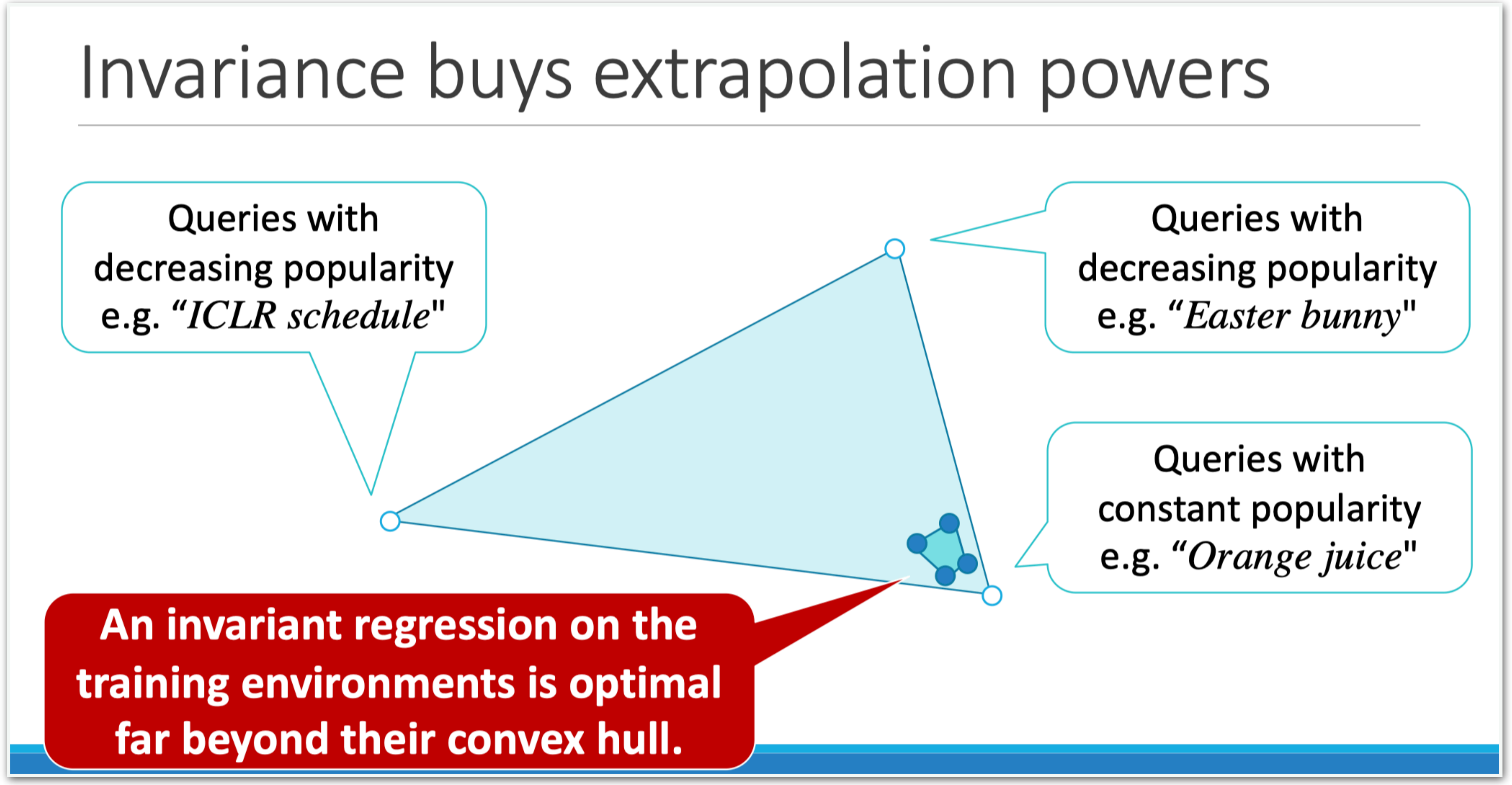


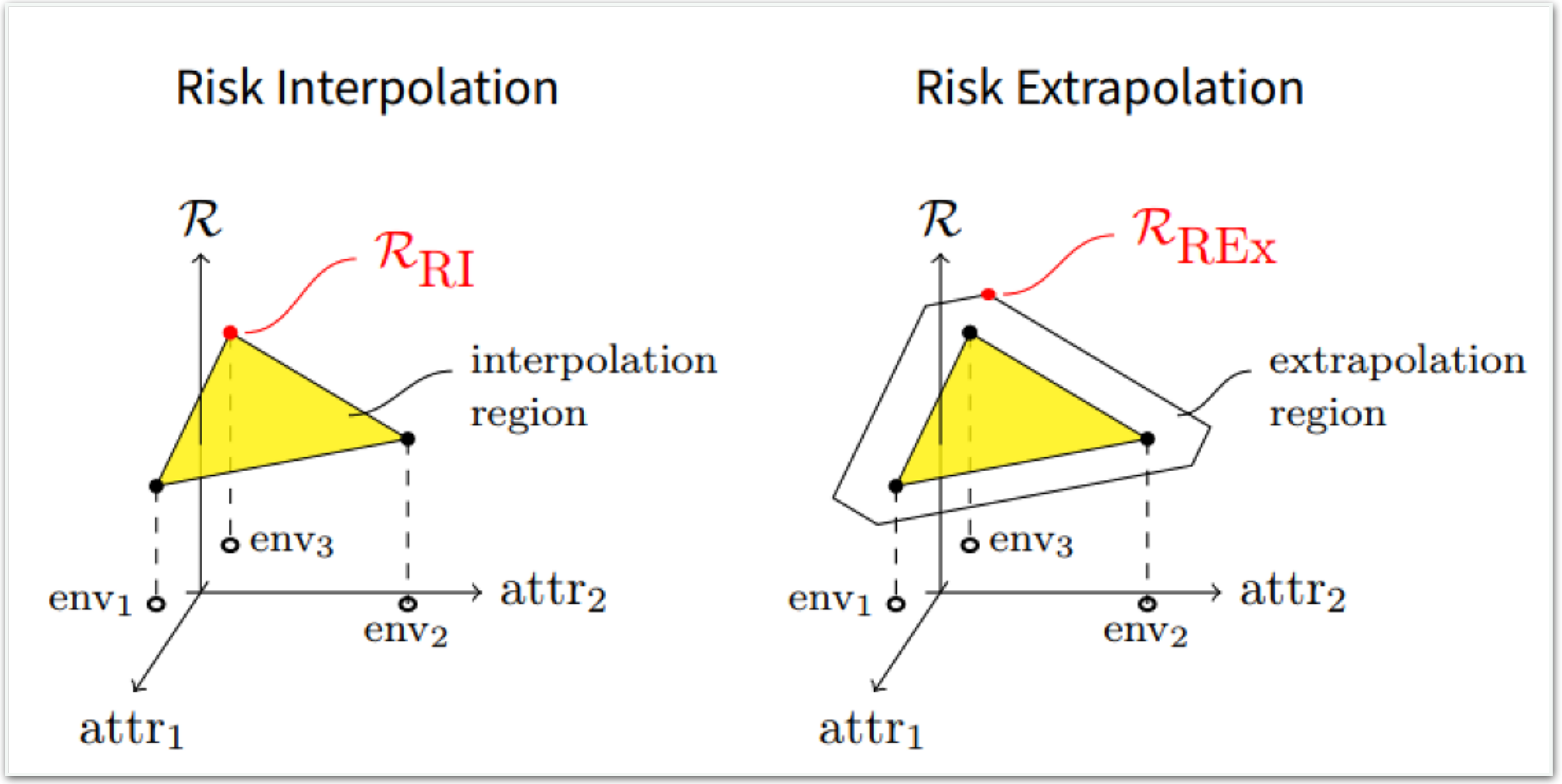
(Arjovsky et al., 2019; Bottou et al., 2019; Krueger et al., 2021)

Robustify MOO objectives

We can introduce **additional** guidance that **directly** enforces extrapolation at certain region.

$$\{\sum_{e\in\mathcal{E}_{\text{tr}}} \lambda_e \mathcal{D}_e \mid \sum_{e\in\mathcal{E}_{\text{tr}}} \lambda_e = 1, \lambda_e \geq 0, \forall e\} \Rightarrow \{\sum_{e\in\mathcal{E}_{\text{tr}}} \lambda_e \mathcal{D}_e \mid \sum_{e\in\mathcal{E}_{\text{tr}}} \lambda_e = 1, \lambda_e \leq 0, \forall e\} \Rightarrow \{\sum_{e\in\mathcal{E}_{\text{tr}}} \lambda_e \mathcal{D}_e \mid \sum_{e\in\mathcal{E}_{\text{tr}}} \lambda_e = 1, \lambda_e \leq -\beta, \forall e\}$$



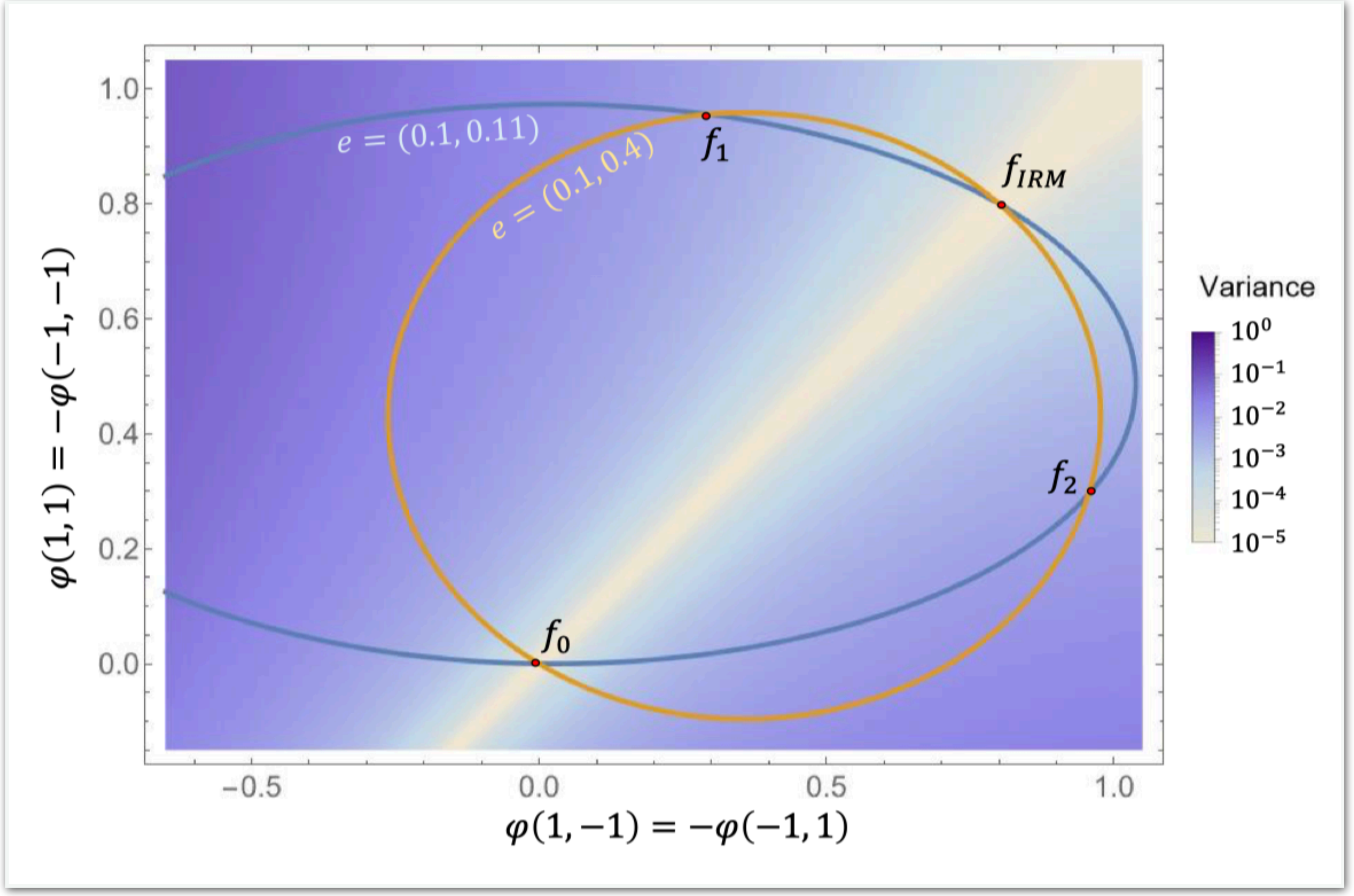


This brings us a new MOO objectives, IRMX: $\min_{f=w\cdot\varphi} \{L_1, L_2, L_{\text{IRM}}, L_{\text{REx}}\}^T$

(Arjovsky et al., 2019; Bottou et al., 2019; Krueger et al., 2021)

PAIR: PAreto Invariant Risk minimization

A PAIRed journey into the adventure of extrapolation: $\min_{f=w\cdot\varphi} \{L_{\text{ERM}}, L_{\text{IRM}}, L_{\text{REx}}\}^T$

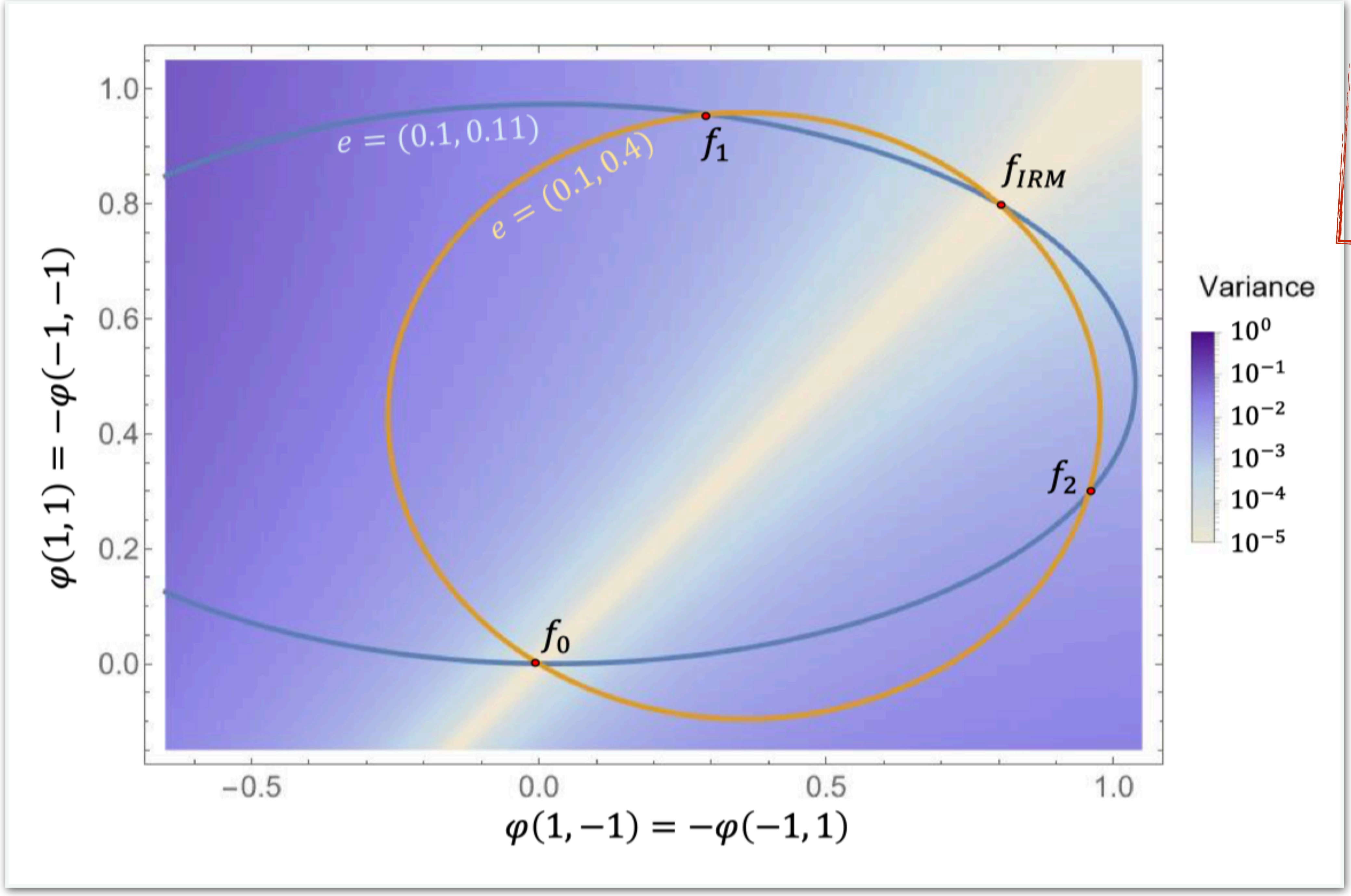


Theoretical results (Informal):

IRMX solves the IRMv1 failures under any environment settings in *(Kamath et al., 2021)*.

PAIR: PAreto Invariant Risk minimization

😋 A PAIRed journey into the adventure of extrapolation: $\min_{f=w\cdot\varphi} \{L_{\mathrm{ERM}}, L_{\mathrm{IRM}}, L_{\mathrm{REx}}\}^T$



IRMX raises more challenges in hp. tuning!

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IRMX solves the IRMv1 failures under any environment settings in *(Kamath et al., 2021)*.

PAIR: PAreto Invariant Risk minimization

IRMX raises more challenges in the optimization:

$$\min_{f=w\cdot\varphi} \{L_{\text{ERM}}, L_{\text{IRM}}, L_{\text{REx}}\}^T$$

- The Pareto front becomes **more complicated**:

PAIR: PAreto Invariant Risk minimization

IRMX raises more challenges in the optimization:

$$\min_{f=w\cdot\varphi} \{L_{\text{ERM}}, L_{\text{IRM}}, L_{\text{REx}}\}^T$$

- The Pareto front becomes **more complicated**:
  ✓ The optimizer needs to be able to reach **any** Pareto optimal solutions!

e.g., MGDA algorithms *(Désidéri, 2012)*

PAIR: PAreto Invariant Risk minimization

IRMX raises more challenges in the optimization:

$$\min_{f=w\cdot\varphi} \{L_{\text{ERM}}, L_{\text{IRM}}, L_{\text{REx}}\}^T$$

- The Pareto front becomes **more complicated**:
  - ✓ The optimizer needs to be able to reach **any** Pareto optimal solutions!
- There can be **multiple** Pareto optimal solutions:

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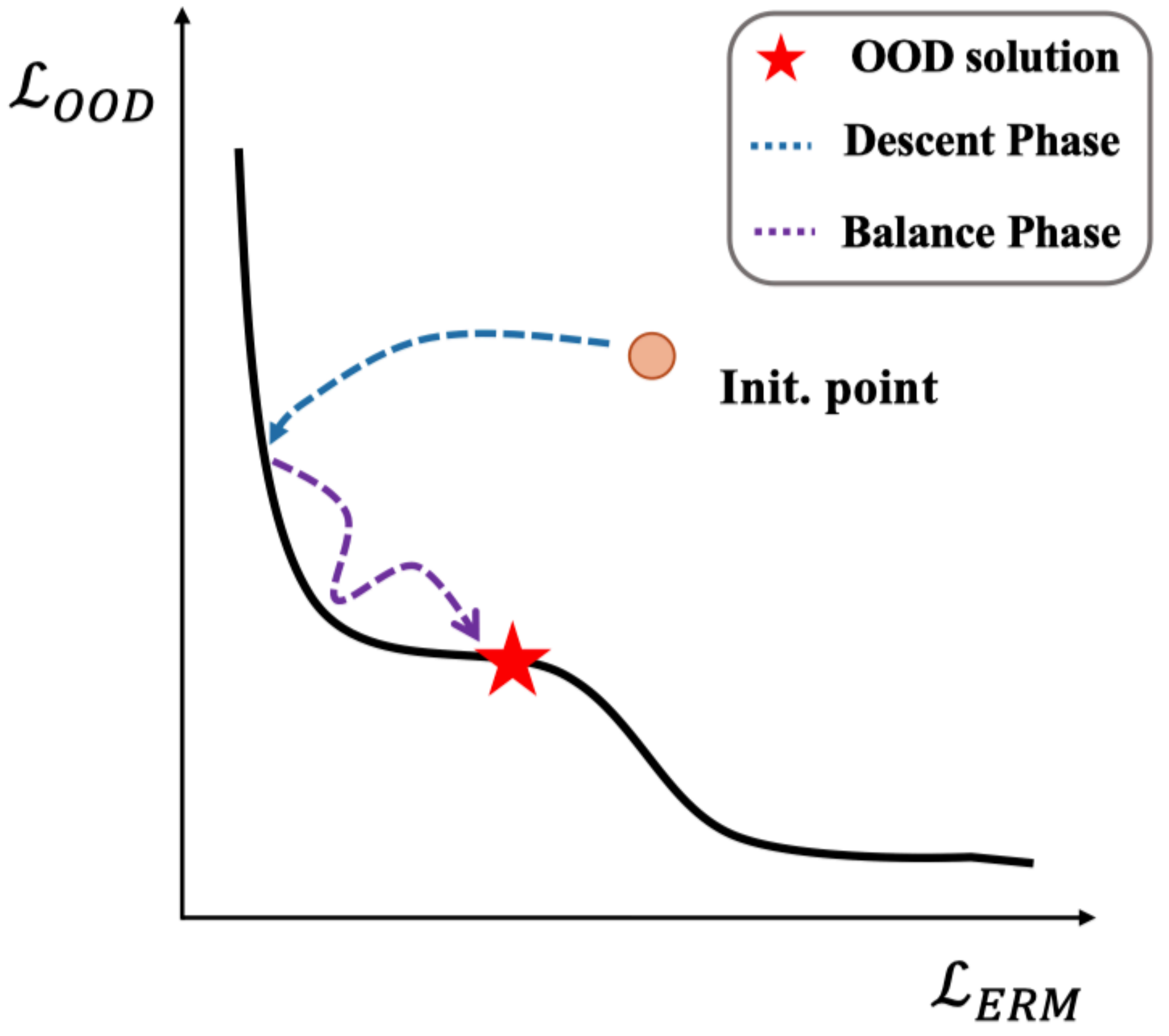
- The Pareto front becomes **more complicated**:
  - ✓ The optimizer needs to be able to reach **any** Pareto optimal solutions!
- There can be **multiple** Pareto optimal solutions:
  - ✓ A **preference** of each objective is required!

Exact Pareto Optimality:

Given a preference $\mathbf{p} = \{p_{\text{ERM}}, p_{\text{IRM}}, p_{\text{REx}}\}^T$ for each objective, a solution $\widehat{\mathbf{L}} = \{\widehat{L}_{\text{ERM}}, \widehat{L}_{\text{IRM}}, \widehat{L}_{\text{REx}}\}^T$ satisfies Exact Pareto Optimality iff. $p_{\text{ERM}}\widehat{L}_{\text{ERM}} = p_{\text{IRM}}\widehat{L}_{\text{IRM}} = p_{\text{REx}}\widehat{L}_{\text{REx}}$.

PAIR: PAreto Invariant Risk minimization



Exact Pareto optimal search

IRMX raises more challenges in the optimization:

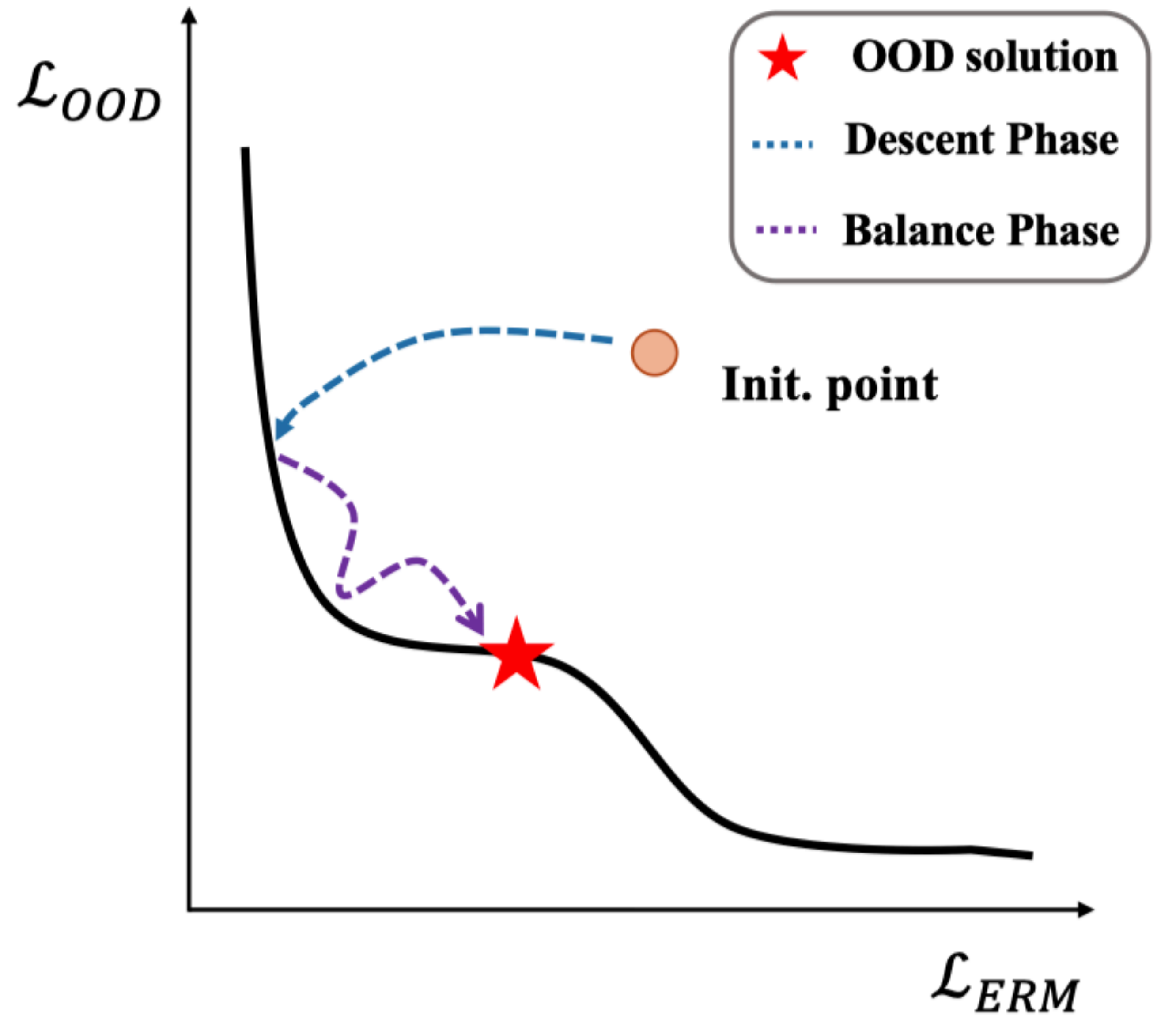
$$\min_{f=w\cdot\varphi} \{L_{\mathrm{ERM}}, L_{\mathrm{IRM}}, L_{\mathrm{REx}}\}^T$$

- The Pareto front becomes **more complicated**:
  - ✓ The optimizer needs to be able to reach **any** Pareto optimal solutions!
- There can be **multiple** Pareto optimal solutions:
  - ✓ A **preference** of each objective is required! ***PAIR-o*** as the OOD optimizer;

Theoretical results (Informal):
Under mild assumptions, let f_{OOD} be the desired OOD solution w.r.t. an underlying preference $\mathbf{p}_{\mathrm{OOD}}$, PAIR-o converges and approximates to f_{OOD} for any approximated $\hat{\mathbf{p}}_{\mathrm{OOD}}$.

(Mahapatra & Rajan 2020)

PAIR: PAreto Invariant Risk minimization



Exact Pareto optimal search

IRMX raises more challenges in the optimization:

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- The Pareto front becomes **more complicated**:
  - ✓ The optimizer needs to be able to reach **any** Pareto optimal solutions!
- There can be **multiple** Pareto optimal solutions:
  - ✓ A **preference** of each objective is required! ***PAIR-o*** as the OOD optimizer;
  - ✓ It also motivates a new model selection criteria, by selecting models that maximally satisfy the Exact Pareto Optimality! ***PAIR-s*** as the OOD model selector;

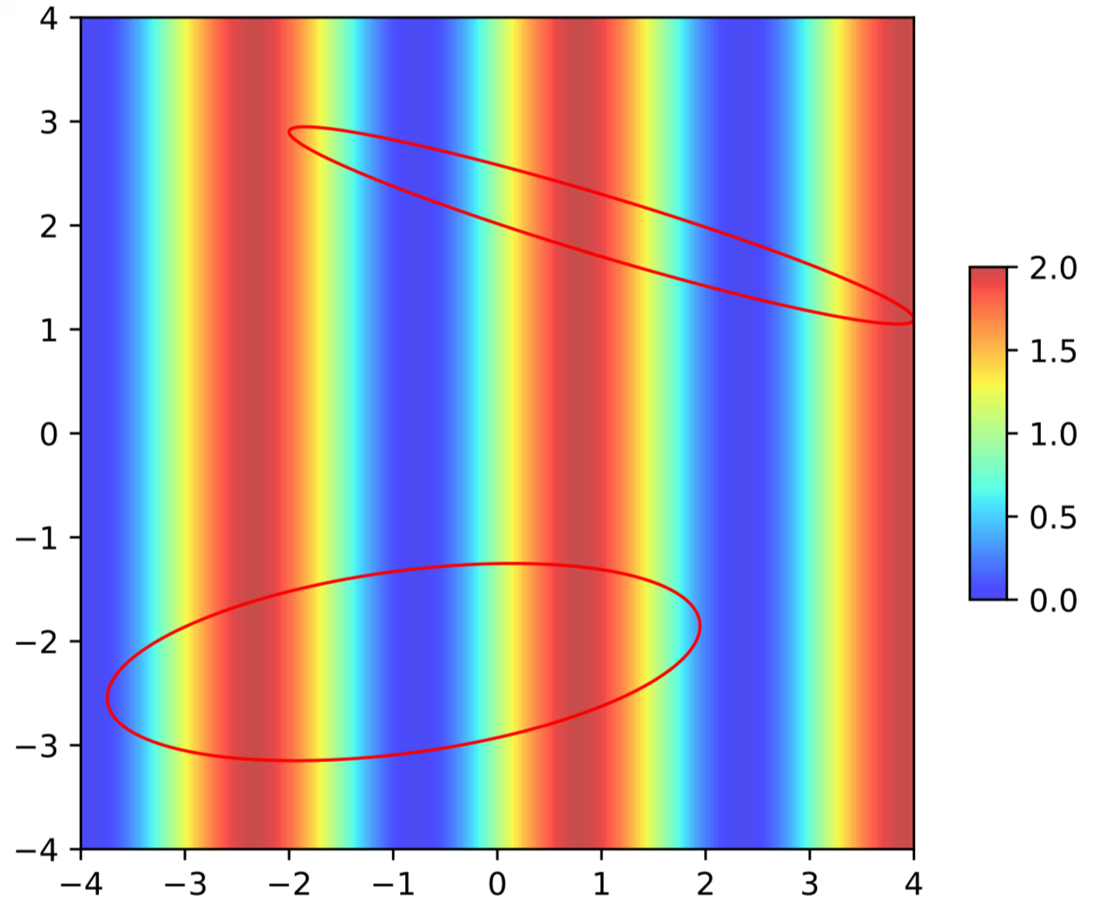
(Gulrajani & Lopez-Paz, 2021)

Causal Invariance Recovery Tests

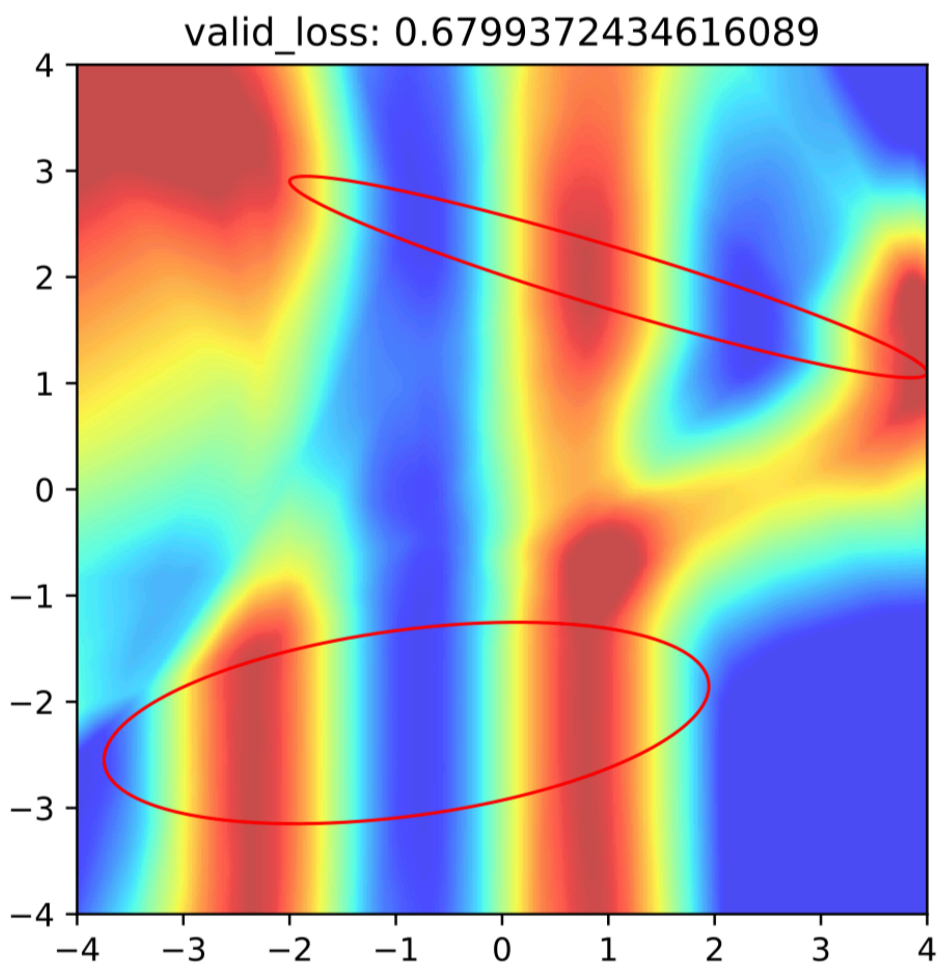
Regression target:
$Y = \sin(X_1) + 1$, only depends on the x-axis;

Training envs:
Two elliptical regions (Gaussian distributions) marked in red;

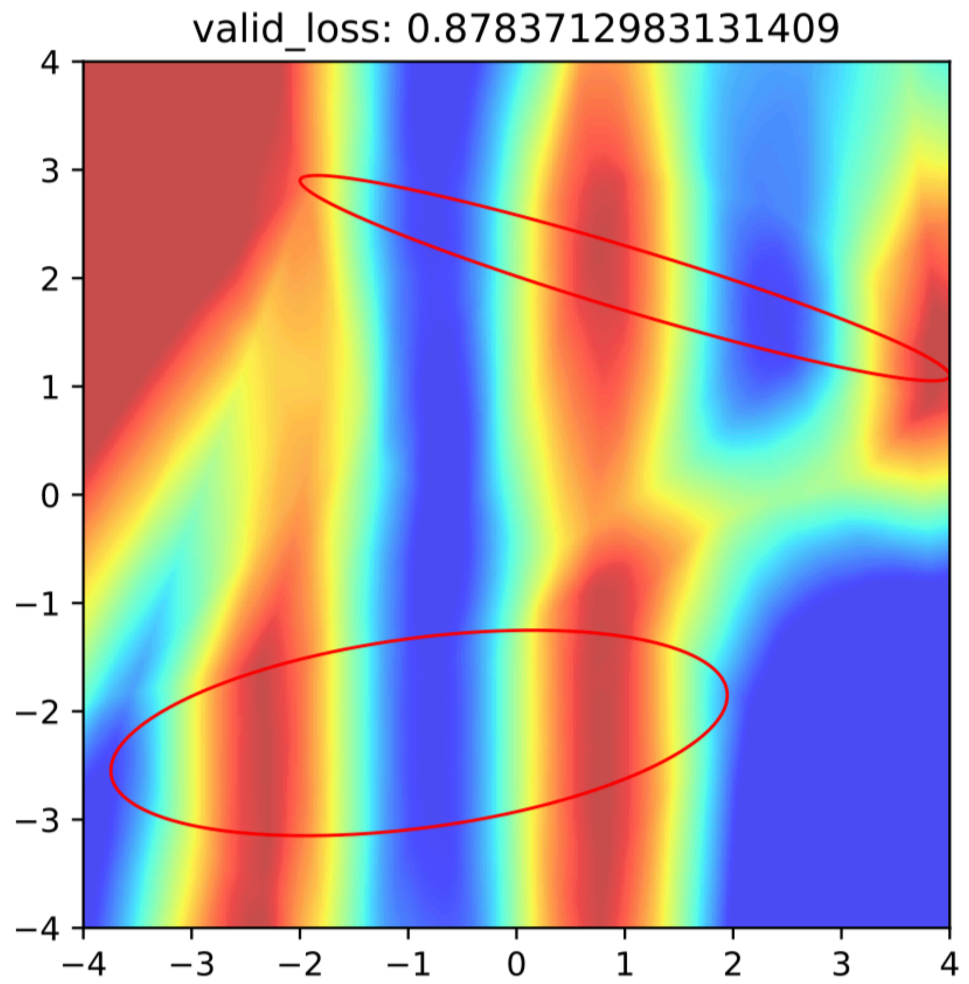
Invariance:
The **overlapped** x-axis region, i.e., $[-2,2]$.



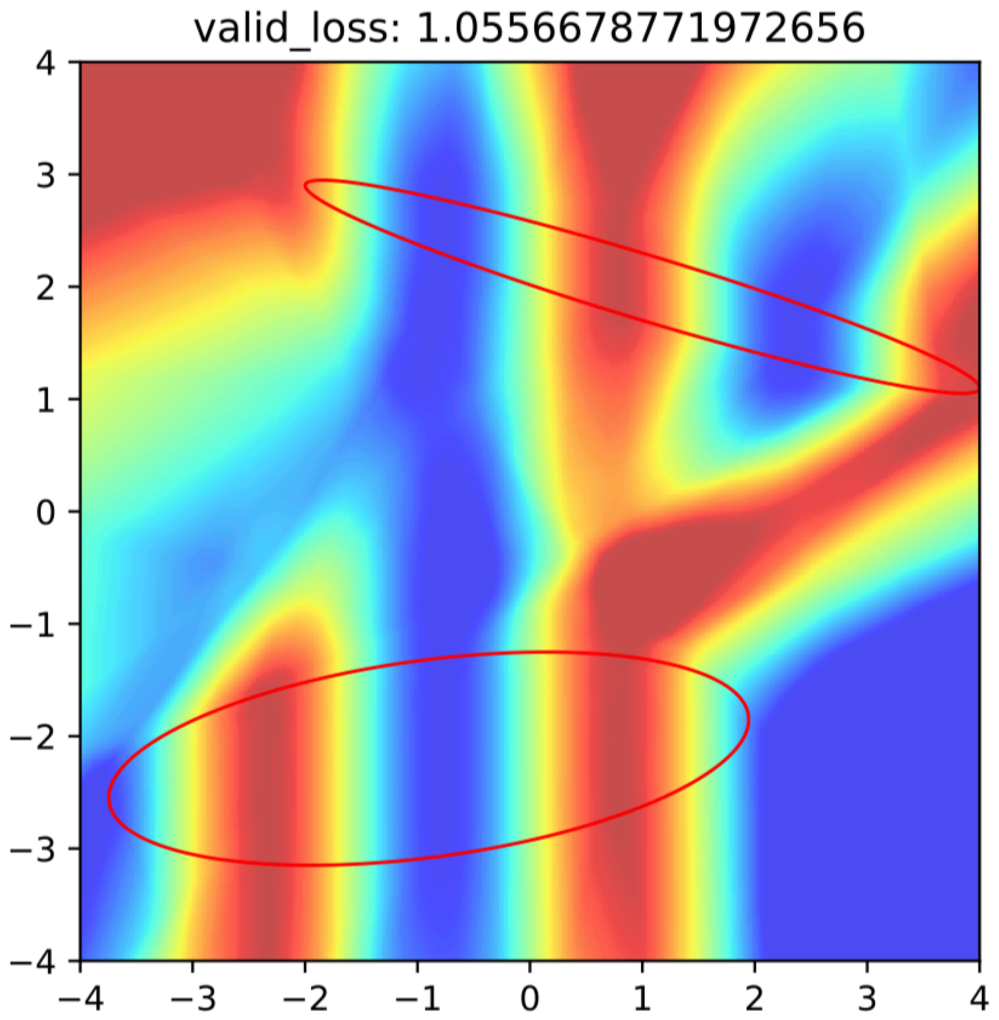
Ground Truth



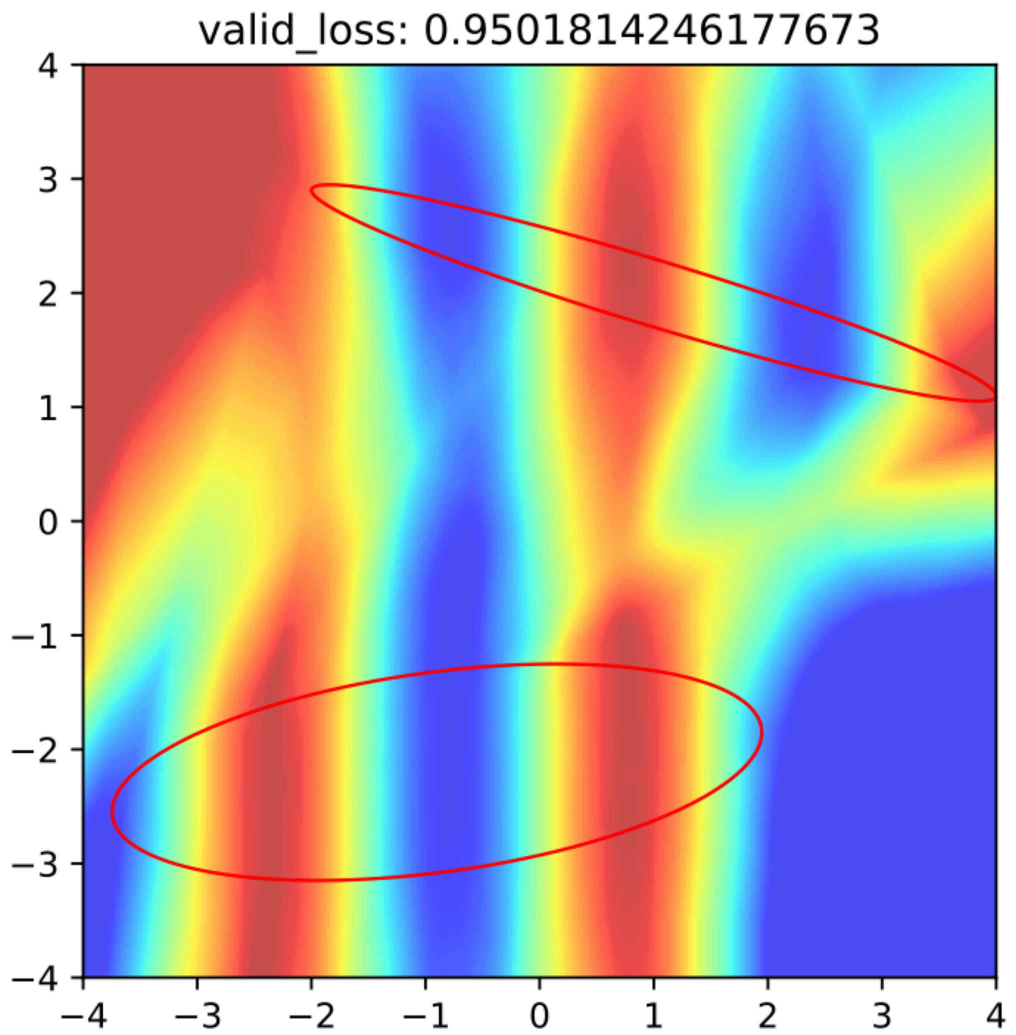
ERM



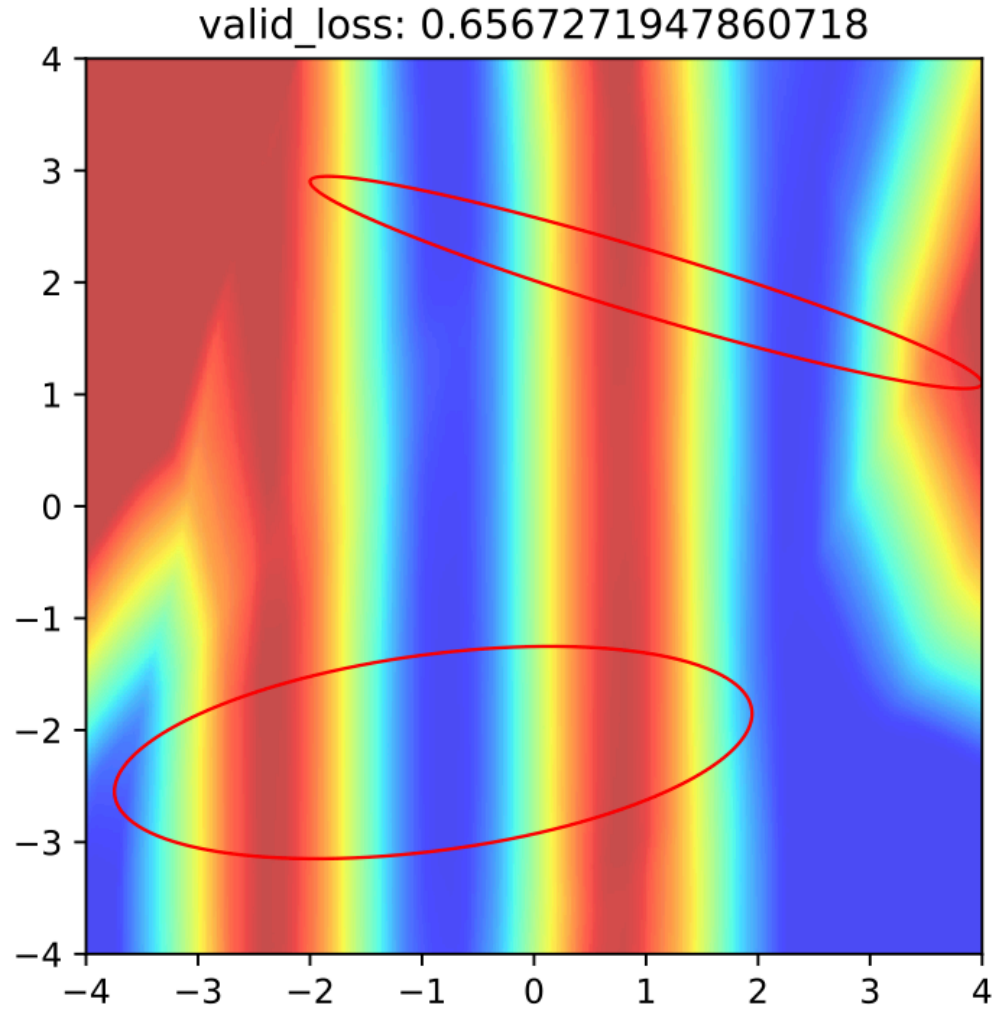
IRMv1



VREx



IRMX



PAIR

PAIR as the optimizer

Table 2: OOD generalization performances on WILDS benchmark.

	CAMELYON17	CIVILCOMMENTS	FMOW	IWILDCAM	POVERTYMAP	RXRX1	AVG. RANK(↓)†
	Avg. acc. (%)	Worst acc. (%)	Worst acc. (%)	Macro F1	Worst Pearson r	Avg. acc. (%)	
ERM	70.3 (±6.4)	56.0 (±3.6)	32.3 (±1.25)	30.8 (±1.3)	0.45 (±0.06)	29.9 (±0.4)	4.50
CORAL	59.5 (±7.7)	65.6 (±1.3)	31.7 (±1.24)	**32.7** (±0.2)	0.44 (±0.07)	28.4 (±0.3)	5.50
GroupDRO	68.4 (±7.3)	70.0 (±2.0)	30.8 (±0.81)	23.8 (±2.0)	0.39 (±0.06)	23.0 (±0.3)	6.83
IRMv1	64.2 (±8.1)	66.3 (±2.1)	30.0 (±1.37)	15.1 (±4.9)	0.43 (±0.07)	8.2 (±0.8)	7.67
V-REx	71.5 (±8.3)	64.9 (±1.2)	27.2 (±0.78)	27.6 (±0.7)	0.40 (±0.06)	7.5 (±0.8)	7.00
Fish	74.3 (±7.7)	73.9 (±0.2)	34.6 (±0.51)	24.8 (±0.7)	0.43 (±0.05)	10.1 (±1.5)	4.33
LISA	**74.7** (±6.1)	70.8 (±1.0)	33.5 (±0.70)	24.0 (±0.5)	**0.48** (±0.07)	**31.9** (±0.8)	2.67
IRMX	67.0 (±6.6)	74.3 (±0.8)	33.7 (±0.78)	26.6 (±0.9)	0.45 (±0.04)	28.7 (±0.2)	4.00
PAIR-o	74.0 (±7.0)	**75.2** (±0.7)	**35.5** (±1.13)	27.9 (±0.7)	0.47 (±0.06)	28.8 (±0.1)	**2.17**

† Averaged rank is reported because of the dataset heterogeneity. A lower rank is better.

PAIR re-empowers IRMv1 and achieves new state-of-the-arts across ***6 challenging realistic datasets***.

PAIR as the model selector

Table 3: OOD generalization performances using DomainBed evaluation protocol.

	PAIR-s	ColoredMNIST †				PACS ‡					TerraIncognita †				
		+90%	+80%	10%	Δ wr.	A	C	P	S	Δ wr.	L100	L38	L43	L46	Δ wr.
ERM		71.0	**73.4**	10.0		87.2	79.5	95.5	76.9		46.7	**41.8**	57.4	39.7	
DANN		71.0	**73.4**	10.0		86.5	79.9	97.1	75.3		46.1	41.2	56.7	35.6	
DANN	✓	71.6	73.3	10.9	+0.9	87.0	81.4	96.8	77.5	+2.2	43.1	41.1	55.2	38.7	+3.1
GroupDRO		72.6	73.1	9.9		87.7	82.1	98.0	79.6		48.4	40.3	57.9	40.0	
GroupDRO	✓	**72.7**	73.2	13.0	+3.1	86.7	**83.2**	**97.8**	81.4	+1.8	48.4	40.3	57.9	40.0	+0.0
IRMv1		72.3	72.6	9.9		82.3	80.8	95.8	78.9		48.4	35.6	55.4	40.1	
IRMv1	✓	67.4	64.8	**24.2**	+14.3	85.3	81.7	97.4	79.7	+0.8	40.4	38.3	48.8	37.0	+1.4
Fishr		72.2	73.1	9.9		**88.4**	82.2	97.7	81.6		49.2	40.6	57.9	40.4	
Fishr	✓	69.1	70.9	22.6	+12.7	87.4	82.6	97.5	**82.2**	+0.6	**51.0**	40.7	**58.2**	**40.8**	+0.3

†Using the training domain validation accuracy. ‡Using the test domain validation accuracy.

PAIR-s substantially improves the worst environment performance of all representative OOD methods up to ***10%***.

Summary

We provided a new understanding of the optimization dilemma in OOD generalization from the Multi-Objective Optimization perspective.

We attributed the failures of OOD optimization to the compromised robustness of relaxed OOD objectives and the unreliable optimization scheme.

We highlighted the importance of trading-off the ERM and OOD objectives and proposed a new optimization scheme PAIR to mitigate the dilemma.

Paper Code

Thank you!

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