Harmonized Cone for Feasible and Non-Conflict Directions in Training Physics-Informed Neural Networks

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*: Equal contribution

Optimization a Feasibility Problem

Find $\mathbf{x}^*$ which satisfies following optimization problem 🤔

$$\min_{\mathbf{x}} \mathbf{0}'\mathbf{x}$$

$$\text{Subject to} \quad g_i(\mathbf{x}) \le b_i \quad \forall i$$
$$h_j(\mathbf{x}) = b_j \quad \forall j$$

Transforming Constraints into Optimization Objectives

$$\min_{\mathbf{x}} \mathbf{0}'\mathbf{x}$$

Subject to $g_i(\mathbf{x}) \leq b_i \quad \forall i$

$h_j(\mathbf{x}) = b_j \quad \forall j$

$=$

$$\min_{\mathbf{x}} \mathbf{0}'\mathbf{x}$$

Subject to $(g_i(\mathbf{x}) - b_i) \leq 0 \quad \forall i$

$\left(h_j(\mathbf{x}) - b_j\right)^2 \leq 0 \quad \forall j$

Lagrangian expression

$$\min_{\mathbf{x}} \max_{\boldsymbol{\lambda}^{\mathbf{g}},\boldsymbol{\lambda}^{\mathbf{h}}} \sum_i \lambda_i^g (g_i(\mathbf{x}) - b_i) + \sum_j \lambda_j^h \left(h_j(\mathbf{x}) - b_j\right)^2$$

Transforming Constraints into Optimization Objectives

$$\min_{\mathbf{x}} \mathbf{0}'\mathbf{x}$$

Subject to $\quad g_i(\mathbf{x}) \le b_i \quad \forall i$

$\qquad\qquad\quad h_j(\mathbf{x}) = b_j \quad \forall j$

=

$$\min_{\mathbf{x}} \mathbf{0}'\mathbf{x}$$

Subject to $\quad (g_i(\mathbf{x}) - b_i) \le 0 \quad \forall i$

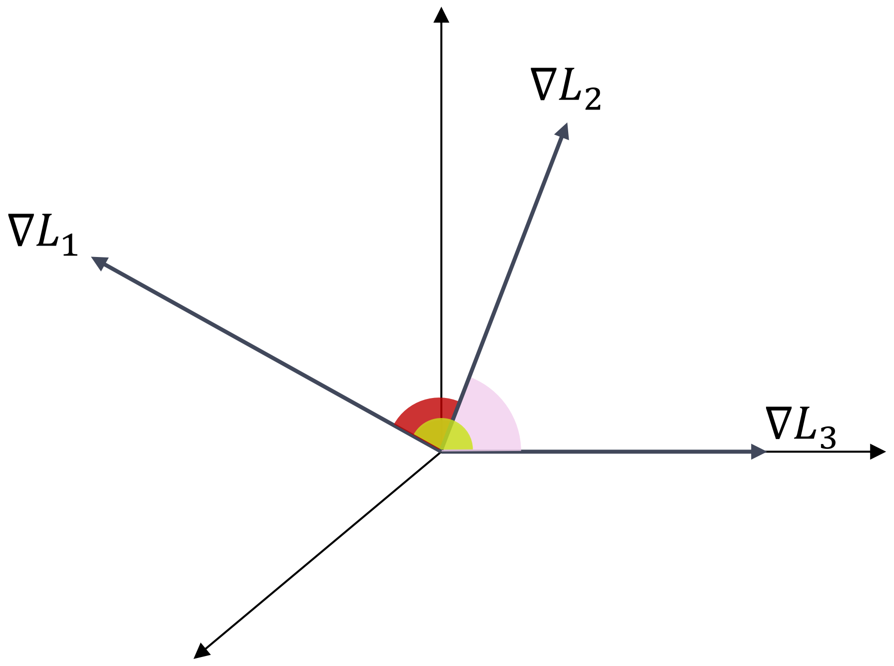
$\qquad\qquad\quad \left(h_j(\mathbf{x}) - b_j\right)^2 \le 0 \quad \forall j$

$$\mathbf{x}^* = \operatorname*{argmin}_{\mathbf{x}} \max_{\boldsymbol{\lambda}} \sum_k \lambda_k L_k$$

Where Should the Gradient Move?

$$\mathbf{x}^* = \underset{\mathbf{x}}{\mathrm{argmin}} \max_{\boldsymbol{\lambda}} \sum_k \lambda_k L_k$$

Find the solution $\mathbf{x}^*$ by **gradient descent**



.. Which direction should be chosen?

The region where the **conditions** required for **optimality are satisfied**!

Constraints Satisfaction as Multi-Objective Optimization

$$\mathbf{x}^* = \underset{\mathbf{x}}{\operatorname{argmin}} \max_{\boldsymbol{\lambda}} \sum_k \lambda_k L_k$$

① Primal Feasibility

$$L_k \leq 0 \quad \forall k$$

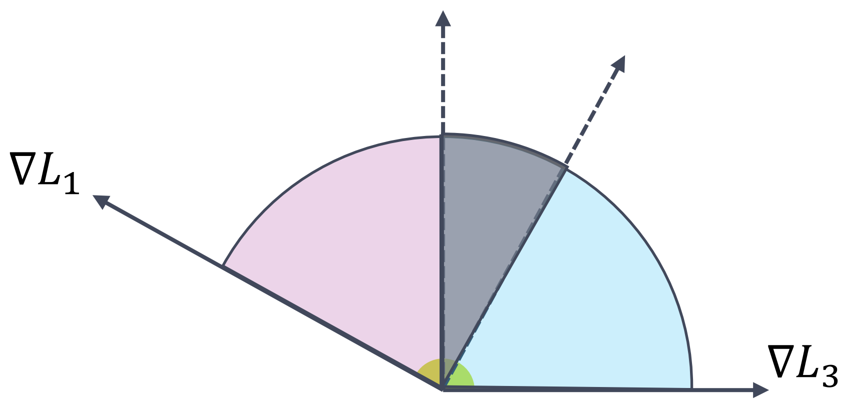
$$\min_{\mathbf{x}} \mathbf{0}'\mathbf{x}$$

Subject to $L_k \leq 0 \quad \forall k$

Find a common optimal solution $\boldsymbol{x}^*$ that satisfies all L_k

∴ Multi-Objective Optimization

Dual Gradient Cone Region



Non-negative Combination of Constraint Gradients

$$\mathbf{x}^* = \underset{\mathbf{x}}{\text{argmin}} \max_{\boldsymbol{\lambda}} \sum_k \lambda_k L_k$$

② Dual Feasiblity

$\lambda_k \geq 0 \quad \forall k$

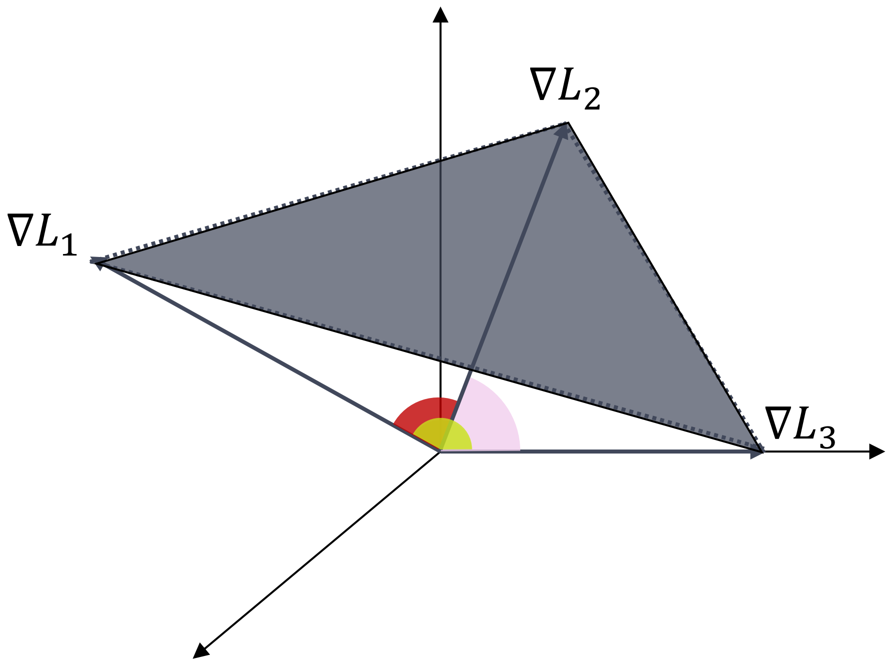
$\max_{\boldsymbol{\lambda}} \boldsymbol{\lambda}' L$

Subject to $\lambda_k \geq 0 \quad \forall k$

Search within the space spanned by non-negative combination of L_k

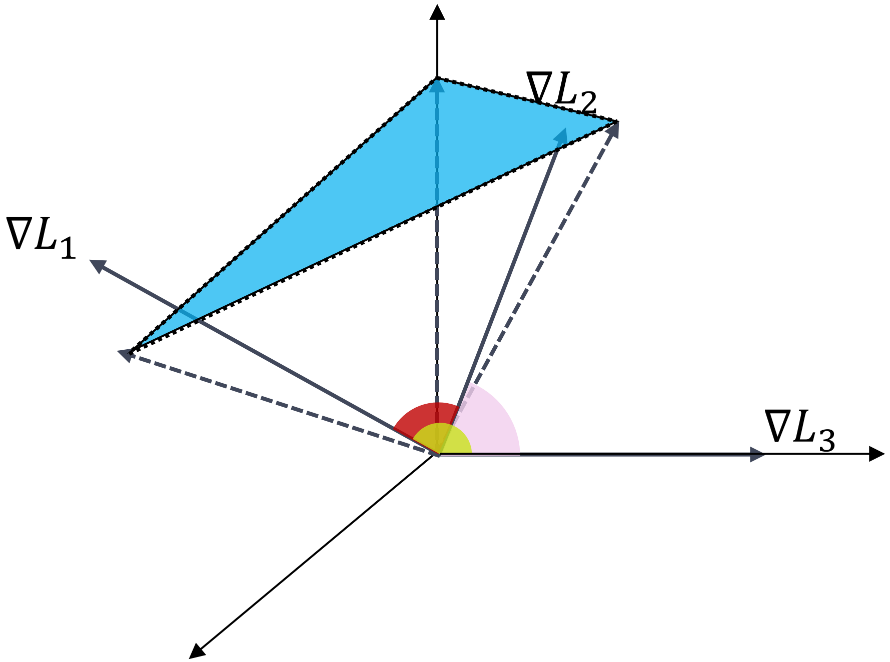
∴ Reweighting Methods

Primal Gradient Cone Region

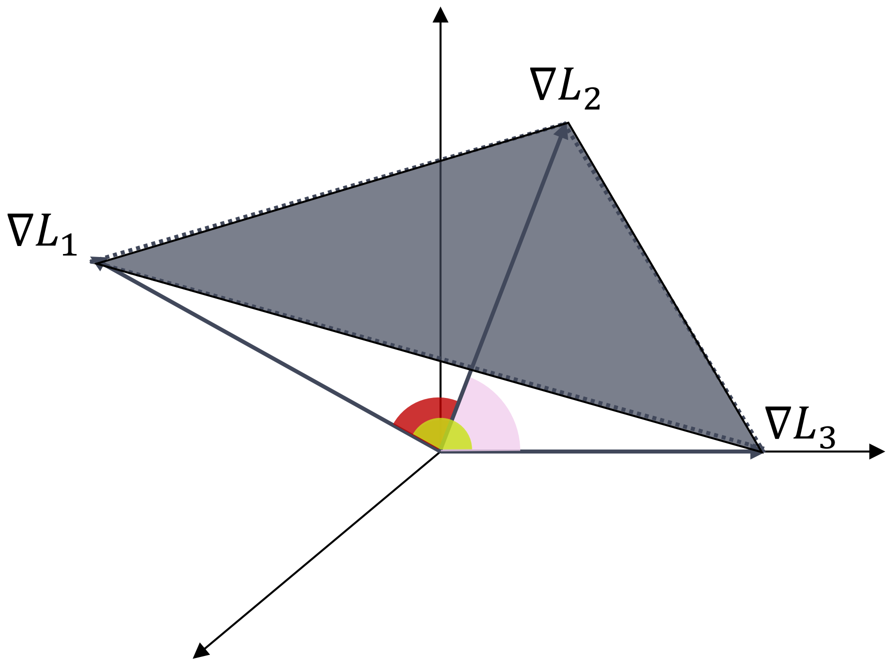


Harmonized Cone: Intersection of Primal and Dual Gradient Cone

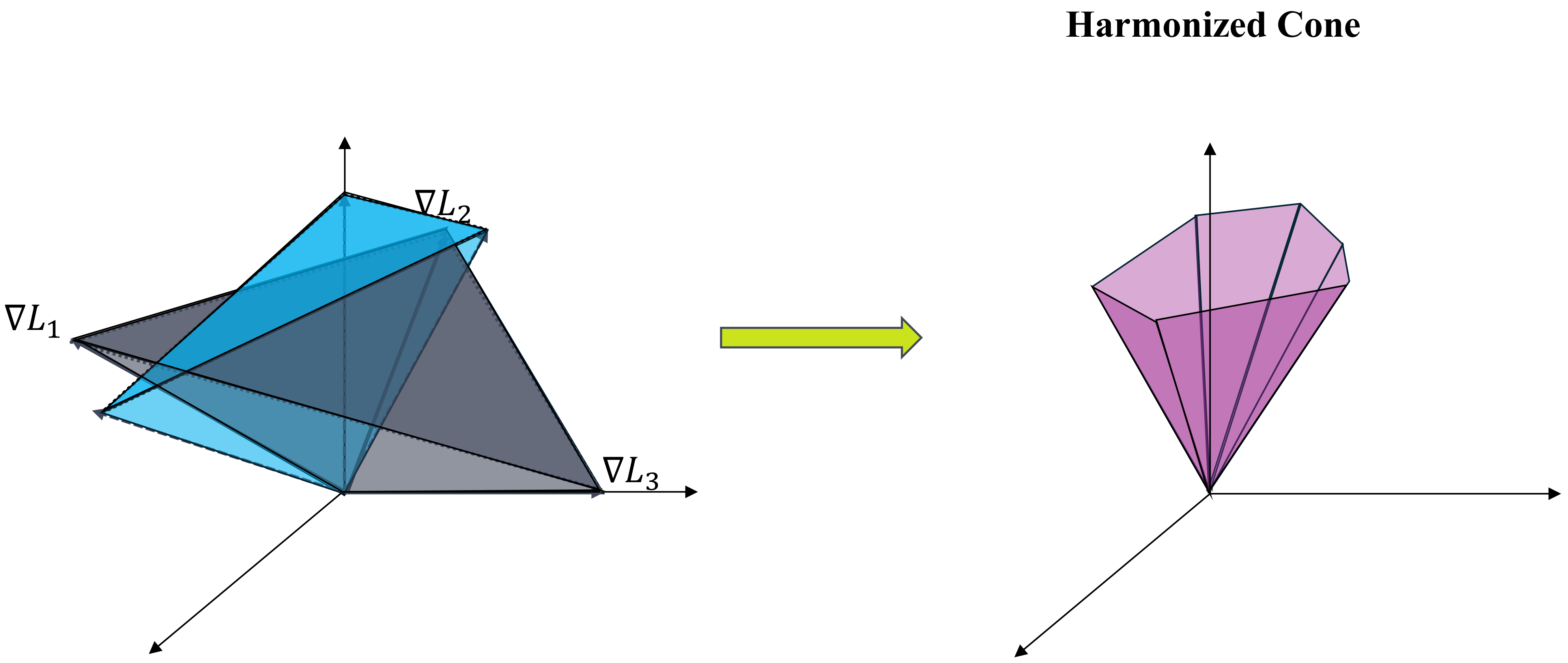
Dual Gradient Cone Region



Primal Gradient Cone Region



Harmonized Cone: Intersection of Primal and Dual Gradient Cone



Come check out our Harmonized Cone!

😎 Scan Me

Paper