Revisiting Scalarization in Multi-Task Learning

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What is Multitask Learning?

Multitask learning:

- Suppose we need to model k different tasks



Conceptual Framework



Model Architecture



Multitask Representation Learning

Multitask learning:

- Train a joint model with multiple heads, where one head ~ one task
 - Pros:
 - Easy to scale to many tasks: adding one more task-specific head
 - Can exploit potential synergies among tasks
 - Cons:
 - Hard to design tailored structures
 - "Negative transfer" could happen due to conflicting tasks



Multitask Representation Learning

Multitask learning:

Multi-objective vector loss:
$$\ell(\{h_i\}_{i=1}^k, g) := \begin{pmatrix} \mathbb{E}_{\mathscr{D}_1^{\mathrm{tr}}}[\ell_1((h_1 \circ g)(X), Y)] \\ \vdots \\ \mathbb{E}_{\mathscr{D}_k^{\mathrm{tr}}}[\ell_k((h_k \circ g)(X), Y)] \end{pmatrix} \in \mathbb{R}^k$$

Note " \leq " is not a total ordering in \mathbb{R}^k for k > 1, so in general we pick a preference vector >

$$w \in \Delta_{k-1} := \left\{ v \in \mathbb{R}^k : \sum_{i=1}^k v_i = 1, v_i \ge 0 \right\}$$

Linear scalarization
$$\min_{g,h_i} \sum_{i=1}^k \frac{w_i}{n_i} \sum_{j=1}^{n_i} \ell_i(h_i \circ g)(x_j^{(i)}), y_j^{(i)})$$

"task-specific header" "shared multitask feature learning"

Multitask Representation Learning



Linear Scalarization for MTL

Linear scalarization:

MTL Loss: \min_{g,h_i}

$$\sum_{i=1}^{k} \frac{w_i}{n_i} \sum_{j=1}^{n_i} \ell_i((h_i \circ g)(x_j^{(i)}), y_j^{(i)})$$

What's the potential problem of simple scalarization?

Not necessarily possible to strike the right balance among multiple tasks



What if we use random weights $w^{(t)} \in \Delta_{k-1}$ at each iteration $t \in [T]$?

A simple starter: simply randomize the combination weighting vector



Pseudo-code:

Algorithm 1 A training iteration in RW methods. The random sampling process is the only difference between RW methods and the existing works. The red line and blue line are the only difference between RLW and RGW methods.

- 1: Input: numbers of tasks T, learning rate η , dataset $\{\mathcal{D}_t\}_{t=1}^T$, weight distribution $p(\tilde{\lambda})$, normalization function f
- 2: Output: task-sharing parameter θ' , task-specific parameters $\{\psi'_t\}_{t=1}^T$

 $\psi'_t = \psi_t - \eta \nabla_{\psi_t} \lambda_t \ell_t(\mathcal{D}_t; \theta, \psi_t) \text{ or } \psi'_t = \psi_t - \eta \nabla_{\psi_t} \ell_t(\mathcal{D}_t; \theta, \psi_t);$

3: **for**
$$t = 1$$
 to T **do**

8: $\theta' = \theta - \eta \sum_{t=1}^{T} \lambda_t g_t;$

9: for t = 1 to T do

4: Compute loss $\ell_t(\mathcal{D}_t; \theta, \psi_t);$

5: Compute gradient
$$g_t = \nabla_{\theta} \ell_t(\mathcal{D}_t; \theta, \psi_t);$$

11: end for

10:

7: Sample weights $\tilde{\boldsymbol{\lambda}}$ from $p(\tilde{\boldsymbol{\lambda}})$ and normalize it into $\boldsymbol{\lambda}$ via f;

▷ Random Sampling

Potential distributions to sample from:

- Uniform, (truncated) Normal, Dirichlet, etc



Variance of gradient norms:







- EW: equal weighting
- RLW: randomized loss weighting

However,

- Unclear this RW (randomized weight) will always converge
- Will it always converge to a Pareto optimal point?

Any other more principled methods to explore the Pareto front? Yes, for batch learning!



"Multiple-Gradient Descent Algorithm (MGDA) for Multi-Objective Optimization", Comptes Rendus Mathématique Désidéri, 2012.

"Multi-Task Learning as Multi-Objective Optimization", NeurIPS'18, Sener and Kolton.

"Gradient Surgery for Multi-Task Learning", NeurIPS'20, Yu et al.

"Conflict-Averse Gradient Descent for Multi-task Learning", NeurIPS'21, Liu et al.

Multiple-Gradient Descent Algorithm

Let $g_i, i \in [k]$ be the gradient for the *k* tasks at a certain iteration First order improvement along direction $d: g_i^{\top} d$

Primal problem:

$$\max_{\|d\|_2 \le 1} \min_{i \in [k]} g_i^\top d$$

Interpretation: finding a common direction d that maximizes the worst-task improvement

Dual problem:

$$\min_{\alpha \in \Delta_{k-1}} \| \sum_{i=1}^{\kappa} \alpha_i g_i \|_2^2$$

1-

 g_1 g_2 MGDA

 $\max_d \min_i g_i^\top d$

s.t. $||d|| \leq 1$

Interpretation: finding a convex combination α of the multiple gradients with minimum \mathcal{C}_2 norm

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Empirical comparisons between linear scalarization vs multiobjective optimization in NNs:



Empirical comparisons between linear scalarization vs multiobjective optimization in NNs:



Observations:

- For large-scale NNs, the closure of the Pareto front seems to be convex
- Deeper and larger models help to enlarge the feasible region (hence achieving Pareto-dominating solutions)

"Do Current Multi-Task Optimization Methods in Deep Learning Even Help?", NeurIPS' 22, Xin et al.

Research Question:

"For NNs, for every Pareto optimal $v \in \mathscr{P}(\mathscr{F})$, does there exists a $w \in \Delta_{k-1}$ such that the optimal solution of the linear scalarization problem corresponds to v?"



- When may MOO help?
- What is the impact of model size?

Multi-task linear network for regression:

- For each task $i \in [k]$, the prediction is given by

$$f_i(x, W, a_i) = x^\top W a_i$$

- Shared input $X \in \mathbb{R}^{n \times p}$, target vector $y_i \in \mathbb{R}^n$, $\forall i \in [k]$, the training loss for task *i*:

$$\ell_i(W, a_i) = \|XWa_i - y_i\|_2^2$$

- Parameter $W \in \mathbb{R}^{p \times q}$, i.e., network width = q, $a_i \in \mathbb{R}^q$ are task-specific parameters

Note:

- For linear networks without loss of generality it suffices to consider a two layer network
- The overall model parameters $\theta = (\{a_i\}_{i=1}^k, W)$. The optimization problem is non-convex for each task i

Phase-transition between over-parametrized and under-parametrized networks:

Over-parametrized regime ($q \ge k$):

Theorem (informal): The network has sufficient capacity to fit all the tasks optimally, and the Pareto front reduces to a singleton $\mathscr{P}(\mathscr{F}) = \{c\}, c \in \mathbb{R}^k$ and hence can be attained via an arbitrary choice of convex coefficient $w \in \Delta_{k-1}$. ℓ_2



"Understanding and Improving Information Transfer in Multi-Task Learning", Zhang et al., ICLR' 20 "Revisiting Scalarization in Multi-Task Learning: A Theoretical Perspective", Hu et al., NeurIPS' 23

Phase-transition between over-parametrized and under-parametrized networks:

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Intuition: let $\hat{y}_i := X(X^T X)^{\dagger} X^T y_i$ be the optimal linear predictor for task i and let $\hat{Y} = [\hat{y}_1, ..., \hat{y}_k] \in \mathbb{R}^{n \times k}$ be a stack of column vectors. Then, due to the ℓ_2 loss, each task-specific loss can be decomposed as



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$$\mathscr{C}_{i}(W, a_{i}) = \|XWa_{i} - y\|_{2}^{2} = \|XWa_{i} - \hat{y}_{i}\|_{2}^{2} + \|\hat{y}_{i} - y_{i}\|_{2}^{2}$$

Note that $\hat{y}_i \in \text{Col}(X)$ is the projection of y_i into the column space spanned by $X \in \mathbb{R}^{n \times p}$, i.e., the optimal linear prediction. Then if the network is wide enough, i.e., $q \ge k$, we can:

- Optimize the network parameter $W \in \mathbb{R}^{p \times q}$ and $\{a_i\}_{i=1}^k \subseteq \mathbb{R}^q$ by allocating one neuron for each task fitting loss \hat{y}_i
- Pick $W \in \mathbb{R}^{p \times q}$ such that W is full-rank
- For every $i \in [k]$, $XWa_i = \hat{y}_i$ has a solution in terms of $a_i \in \mathbb{R}^q$ (because $q \ge k$ and $\hat{y}_i \in Col(X) = Col(XW)$)
- Putting all together, we have $\|XWa_i \hat{y}_i\|_2^2 = 0$ and $c_i = \|\hat{y}_i y_i\|_2^2$, $\forall i \in [k]$

Under-parametrized regime (q < k):

Theorem (informal): We focus on two extremal cases:

- Extremely under-parametrized (q = 1): Linear scalarization suffices, i.e., full-exploration of the Pareto front, if and only if $G := \hat{Y}^{\top}\hat{Y}$ is doubly non-negative, i.e., the inner products for all task pairs \hat{y}_i and \hat{y}_j are non-negative, up to negating the directions of some $\hat{y}_i, i \in [k]$
- Mildly under-parametrized (q = k 1): Linear scalarization suffices if and only if $Q = G^{-1}$ is doubly non-negative, up to negating the directions of some $\hat{y}_i, i \in [k]$

Remark:

- This means that in general under the under-parametrized regime, linear scalarization is not sufficient of full exploration
- *G* and *Q* could be understood as a notion of "task-similarity" task similarity is model-dependent!, i.e., $G_{ij} = \langle \hat{y}_i, \hat{y}_j \rangle$
- Sufficient and necessary conditions for the general case of 1 < q < k 1 still open

Geometric intuition of the under-parametrized regime:

Notation: let $\hat{y}_i := X(X^\top X)^{\dagger} X^\top y_i$ be the optimal linear predictor for task i and let $\hat{Y} = [\hat{y}_1, ..., \hat{y}_k] \in \mathbb{R}^{n \times k}$ be a stack of column vectors.

For every fixed $W \in \mathbb{R}^{p \times q}$, $Z = XW \in \mathbb{R}^{n \times q}$ are the linear representations learned by NNs. Each task-specific head admits an optimal solution $a_i^* = (Z^T Z)^{\dagger} Z^T \hat{y}_i$.

Hence, each task-specific loss \mathcal{C}_i could be simplified to

$$\min_{Z=XW} \|Z(Z^{\mathsf{T}}Z)^{\dagger}Z^{\mathsf{T}}\hat{y}_{i} - \hat{y}_{i}\|_{2}^{2}$$

Let $P_Z := Z(Z^T Z)^{\dagger} Z^T$ be the projection matrix under a fixed linear representation Z = XW, then the MOO optimization problem becomes

$$\max_{P_Z} \quad (\hat{y}_1^{\mathsf{T}} P_Z \hat{y}_1, \dots, \hat{y}_k^{\mathsf{T}} P_Z \hat{y}_k)$$

Geometric intuition of the under-parametrized regime: Let $P_Z := Z(Z^T Z)^{\dagger} Z^T$ be the projection matrix under a fixed linear representation Z = XW, then the MOO optimization problem becomes

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To illustrate the idea, let's consider the case q = 1 and $P_Z = vv^{\top}$ with $||v||_2 = 1$. Define $s_i = \hat{y}_i^{\top} v$ and $s = \hat{Y}^{\top} v \in \mathbb{R}^k$.

$$\max_{P_Z} \quad (\hat{y}_1^{\mathsf{T}} P_Z \hat{y}_1, \dots, \hat{y}_k^{\mathsf{T}} P_Z \hat{y}_k) \iff \max_{v} \quad (s_1^2, \dots, s_k^2)$$

But,
$$s^{\mathsf{T}} \left(\hat{Y}^{\mathsf{T}} \hat{Y} \right)^{\dagger} s = v^{\mathsf{T}} \hat{Y} \left(\hat{Y}^{\mathsf{T}} \hat{Y} \right)^{\dagger} \hat{Y}^{\mathsf{T}} v \le 1$$

This is a function of a k-dim ellipsoid!

Geometric intuition of the under-parametrized regime:

$$\max_{P_Z} \quad (\hat{y}_1^\top P_Z \hat{y}_1, \dots, \hat{y}_k^\top P_Z \hat{y}_k) \iff \max_{v} \quad (s_1^2, \dots, s_k^2)$$
$$s^\top \left(\hat{Y}^\top \hat{Y} \right)^\dagger s = v^\top \hat{Y} \left(\hat{Y}^\top \hat{Y} \right)^\dagger \hat{Y}^\top v \le 1$$

and

This is a function of a k-dim ellipsoid!

Furthermore, a few observations:

- The objective is invariant under negation of $\hat{y}_i, i \in [k]$
- Under negation, there are 2^k different configurations, each configuration corresponds to an (potentially degenerated) ellipsoid
- The feasible region \mathscr{F} will be the union of 2^k ellipsoid

Geometric intuition of the under-parametrized regime:

Let $P_Z := Z(Z^T Z)^{\dagger} Z^T$ be the projection matrix under a fixed linear representation Z = XW, then the MOO optimization problem becomes

$$\max_{P_Z} \quad (\hat{y}_1 P_Z \hat{y}_1, \dots, \hat{y}_k P_Z \hat{y}_k)$$



Multi-task non-linear network for regression:

Theorem (informal): If $q \ge nk$, then there exists a network that has sufficient capacity to fit all the tasks optimally, and the Pareto front reduces to a singleton $\mathscr{P}(\mathscr{F}) = \{c\}, c \in \mathbb{R}^k$ and hence can be attained via an arbitrary choice of convex coefficient $w \in \Delta_{k-1}$. Remark:

- This upper bound is potentially very loose; ideally we would like an upper bound on the width *q* that only depends on the number of tasks *k* not the number of data points *n*
- No lower bound known, i.e., is there a trade-off problem in general for under-parametrized nonlinear NNs?

NN-Width	Linear NNs	Nonlinear NNs
Upper bound (sufficient)	k	nk
Lower bound (necessary)	k	?

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Empirical evidence:



(a) MGDA with multiple initializations



(b) MGDA-UB with multiple initializations

Under-parametrized regime (q < k): how to rescue?

Randomization!

Randomization \approx Convexification

Given two under-parametrized networks f_0 and f_1 , we can construct a randomized network as follows:

$$f(x) = \begin{cases} f_0(x) & \text{if } S \leq t \\ f_1(x) & \text{o.w.} \end{cases}$$

where $t \in [0,1]$ and $S \sim U(0,1)$ is a uniform RV over (0,1). Then

 $\mathbb{E}_{S,X,Y}[\ell(f(X),Y)] = t\mathbb{E}_{X,Y}[\ell(f_0(X),Y)] + (1-t)\mathbb{E}_{X,Y}[\ell(f_1(X),Y)]$

By choosing different $t \in (0,1)$ we can interpolate and hence convexity any given feasible region \mathcal{F} .

$$\mathscr{F}_{S} = \operatorname{conv}(\mathscr{F}) \longrightarrow \mathscr{P}(\mathscr{F}_{S}) = \mathscr{P}(\operatorname{conv}(\mathscr{F}))$$

How to Rescue?

Under-parametrized regime (q < k): how to rescue?

Chebyshev scalarization:
$$w \in \Delta_{k-1} := \left\{ v \in \mathbb{R}^k : \sum_{i=1}^k v_i = 1, v_i \ge 0 \right\}$$

Chebyshev scalarization
 $\min_{g,h_i} \max_{i \in [k]} \frac{W_i}{n_i} \sum_{j=1}^{n_i} \ell_i((h_i \circ g)(x_j^{(i)}), y_j^{(i)})$

Theorem (Choo & Atkins, 1983): Any feasible solution that is weakly Pareto optimal if and only if it is a solution for a weighted Chebyshev problem under some preference vector $w \in \Delta_{k-1}$.

"Proper Efficiency in Nonconvex Multicriterion Programming", Choo and Atkins, Mathematics of Operation Research, 1983
"A Unifying Perspective on Multi-Calibration: Game Dynamics for Multi-Objective Learning", Haghtalab et al., NeurIPS' 23
"Robust Multi-Task Learning with Excess Risks", He et al., ICML' 24
"Smooth Tchebycheff Scalarization for Multi-Objective Optimization", Lin et al., ICML' 24



Solving the Chebyshev scalarization problem with online mirror descent:

$$\min_{\theta \in \Theta} \max_{i \in [k]} \frac{1}{n_i} \sum_{j=1}^{n_i} w_i \mathcal{C}_i(f_\theta(x_j^{(i)}), y_j^{(i)})$$

$$\min_{\theta \in \Theta} \max_{\lambda \in \Delta_{k-1}} \frac{\lambda_i}{n_i} \sum_{j=1}^{n_i} w_i \mathcal{C}_i(f_\theta(x_j^{(i)}), y_j^{(i)})$$

Upon receiving a batch $Z^{(t)} = \{X^{(t)}, Y^{(t)}\}$:

- Apply (projected) gradient descent to optimize the primal variable: model parameter $\theta\in\Theta$
- Apply exponentiated gradient / multiplicative weight update / hedging algorithm to optimize the dual variable: $\lambda \in \Delta_{k-1}$

Solving the Chebyshev scalarization problem with online mirror descent:

$$\min_{\theta \in \Theta} \max_{\lambda \in \Delta_{k-1}} \frac{\lambda_i}{n_i} \sum_{j=1}^{n_i} w_i \ell_i(f_{\theta}(x_j^{(i)}), y_j^{(i)})$$

Primal update:

$$\boldsymbol{\theta}^{(t+1)} = \Pi_{\Theta} \left(\boldsymbol{\theta}^{(t)} - \eta_{\boldsymbol{\theta}} \boldsymbol{\lambda}^{(t)} \circ \mathbf{w} \circ \nabla \mathbf{f}(\boldsymbol{\theta}^{(t)}) \right)$$

Dual update:

$$\lambda_i^{(t+1)} = \frac{\lambda_i^{(t)} \exp\left(\eta_{\lambda} w_i f_i(\boldsymbol{\theta}^{(t)})\right)}{\sum_{j=1}^m \lambda_j^{(t)} \exp\left(\eta_{\lambda} w_j f_j(\boldsymbol{\theta}^{(t)})\right)}$$

At the end of *T* iterations, we have a sequence of model parameters $\theta^{(1)}, \ldots, \theta^{(T)}$, how to combine them?

Our solution: Adaptive online-to-batch conversion:

- Maintain an active set of PO solutions during the algorithm
- Credit assignment: weight $\gamma^{(t)}$ of each solution $\theta^{(t)} \propto 1 + \#$ of intermediate solutions dominated by it
- For dominated solutions, weight $\gamma^{(t)} = 0$

$$\theta^* := \frac{1}{T} \sum_{t=1}^T \gamma^{(t)} \theta^{(t)}$$



Under the following assumptions:

- Convexity: each $f_i(\theta)$ is convex in $\theta \in \mathbb{R}^d$
- Bounded feasible region: $\forall \theta \in \Theta, \|\theta\|_2 \leq R_{\theta}$
- Bounded gradients: $\forall i \in [k], \forall \theta \in \Theta, \|\nabla_{\theta} f_i(\theta)\|_2 \leq L$

$$\text{TCH}(\theta; w) := \max_{i \in [k]} \frac{1}{n_i} \sum_{j=1}^{n_i} w_i \ell_i(f_{\theta}(x_j^{(i)}), y_j^{(i)})$$

Theorem (convergence): under the above assumptions and the adaptive online mirror descent with learning rate $\eta = O(\sqrt{1/T})$, the algorithm converges as follows:

$$\mathbb{E}\left[\mathrm{TCH}(\theta^*; w)\right] - \min_{\theta \in \Theta} \mathrm{TCH}(\theta; w) \le O\left(\frac{d}{\sqrt{T}} + \frac{\sqrt{\log k}}{\sqrt{T}}\right)$$

Controlled PO solution:



Convergence speed and stability:



MNIST Rotation

Convergence speed and stability:

CIFAR10 Rotation



LibMoon: A Gradient-based MultiObjective OptimizatioN Library in PyTorch



LibMOON: A Gradient-based MultiObjective OptimizatioN Library in PyTorch

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LibM00N is an open-source library built on <u>PyTorch</u> for gradient based MultiObjective (MOO). See the <u>latest</u> <u>documentation</u> for detailed introductions and API instructions.

Star or fork us on GitHub — it motivates us a lot!

Method	Solution Property	Complexity	Pref.
EPO [16]	Exact solutions	$O(m^2 nK)$	\checkmark
HVGrad [37]	Solutions with maximal HV	$O(m^2 n K^2)$	x
MGDA-UB [12]	Random solutions	$O(m^2 nK)$	x
MOO-SVGD [17]	Diversity by particles repulsion	$O(m^2 n K^2)$	×
PMGDA [38]	Solutions under specific demands	$O(m^2 nK)$	\checkmark
PMTL [13]	Solutions in sectors	$O(m^2 n K^2)$	x
Random [39]	Random solutions	$O(m^2 nK)$	x
Agg-LS [36]	Convex part of a PF	O(mnK)	\checkmark
Agg-Tche [29]	Exact solutions	O(mnK)	\checkmark
Agg-mTche [40]	Exact solutions	O(mnK)	\checkmark
Agg-PBI [29]	Approximate exact solutions	O(mnK)	\checkmark
Agg-COSMOS [33]	Approximate exact solutions	O(mnK)	\checkmark
Agg-SmoothTche [22]	Approximate exact solutions	O(mnK)	\checkmark

m: number of objectives. n: number of decision variables. K: number of subproblems. m is usually small (e.g., 2-4), K is relatively large (e.g., 20-40), and n is particularly large (e.g., 10,000). Therefore, m^2 is not a big concern, while K^2 and n^2 are big concerns. Complexity is for time complexity, and Pref. denotes whether this method is preference-based or not.



"LibMOON: A Gradient-based MultiObjective OptimizatioN Library in PyTorch", Zhang et al., NeurIPS' 24 D&B Track Github repo: <u>https://github.com/xzhang2523/libmoon</u>

Summary

Insights and Implications for us:

- The problem of linear scalarization vs MOO for multitask learning is model-dependent
- Good news: with sufficient capacity of the networks, linear scalarization can represent every Pareto optimal solution
- For linear MTL models under regression tasks we identify a precise phase-transition q = k
- For nonlinear MTL models we have a (loose) upper bound q = nk
- For under-parametrized models, we can use Chebyshev scalarization to control the converged PO solution

Open questions:

- How about linear MTL for classification?
- Is there a similar phase transition phenomenon for nonlinear MTL models?
- Pareto-set learning: a single model/algorithm to learn all the diverse PO solutions simultaneously

Thanks!



Reference:

- 1. Revisiting Scalarization in Multi-Task Learning: A Theoretical Perspective, NeurIPS' 23
- 2. Robust Multi-Task Learning with Excess Risks, ICML' 24
- 3. LibMOON: A Gradient-based MultiObjective OptimizatioN Library in PyTorch, NeurIPS' 24 D&B Track
- Online Mirror Descent for Tchebycheff Scalarization in Multi-Objective Optimization, arXiv: 2410.21764