On Implicit Bias in Overparameterized Bilevel Optimization

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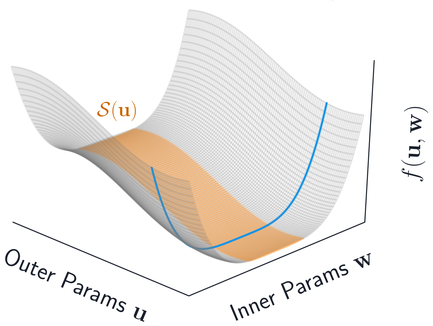
Motivation

- Bilevel problems involve nested optimization, with an outer obj solved subject to the optimality of an inner obj:

$$\mathbf{u}^\star \in \text{“}\operatorname*{argmin}_{\mathbf{u}\in\mathcal{U}}\text{”}\, F(\mathbf{u}, \mathbf{w}^\star)$$
$$\mathbf{w}^\star \in \mathcal{S}(\mathbf{u}^\star) = \operatorname*{argmin}_{\mathbf{w}\in\mathcal{W}} f(\mathbf{u}^\star, \mathbf{w})$$

- **Examples**: hyperparameter optimization (HO), dataset distillation, meta-learning, NAS, and GANs.



Most work assumes that the inner/outer objectives have unique solutions, but in practice, at least one of them is underspecified → non-unique solutions.

Gradient-Based Bilevel Optimization (BLO)

- Gradient-based BLO requires the total gradient of the outer objective w.r.t. the outer parameters, which we call the *hypergradient* (as in HO). For a given solution $\mathbf{w}^* \in \mathcal{S}(\mathbf{u})$, which is called a *best-response* to $\mathbf{u}$: $\frac{dF(\mathbf{u},\mathbf{w}^*)}{d\mathbf{u}} = \frac{\partial F}{\partial \mathbf{u}} + \frac{\partial F}{\partial \mathbf{w}^*}\frac{\partial \mathbf{w}^*}{\partial \mathbf{u}}$

Warm-Start vs Cold-Start

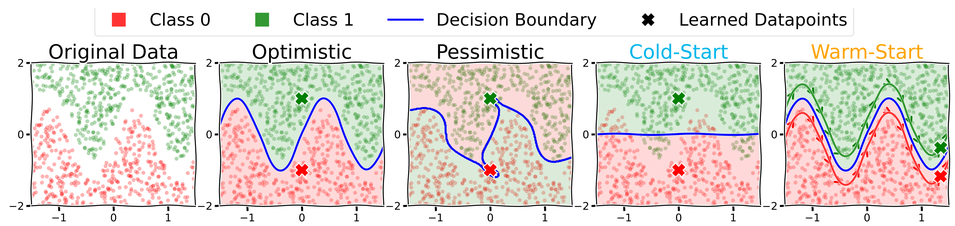
- **Cold-start:** re-initialize $\mathbf{w}$ and run inner optimization to convergence for each hypergradient computation
- **Warm-start:** jointly optimize $\mathbf{w}$ and $\mathbf{u}$ online, alternating gradient steps with their respective objectives
- Let $\Xi^{(T)}(\mathbf{u}, \mathbf{w})$ denote T steps of inner optimization

Method	Inner Update
Cold-Start	$\mathbf{w}^\star_{k+1} = \Xi^{(\infty)}(\mathbf{u}_{k+1}, \mathbf{w}_0)$
Full Warm-Start	$\mathbf{w}^\star_{k+1} = \Xi^{(\infty)}(\mathbf{u}_{k+1}, \mathbf{w}^\star_k)$
Partial Warm-Start	$\mathbf{w}^\star_{k+1} = \Xi^{(T)}(\mathbf{u}_{k+1}, \mathbf{w}^\star_k)$

Theory

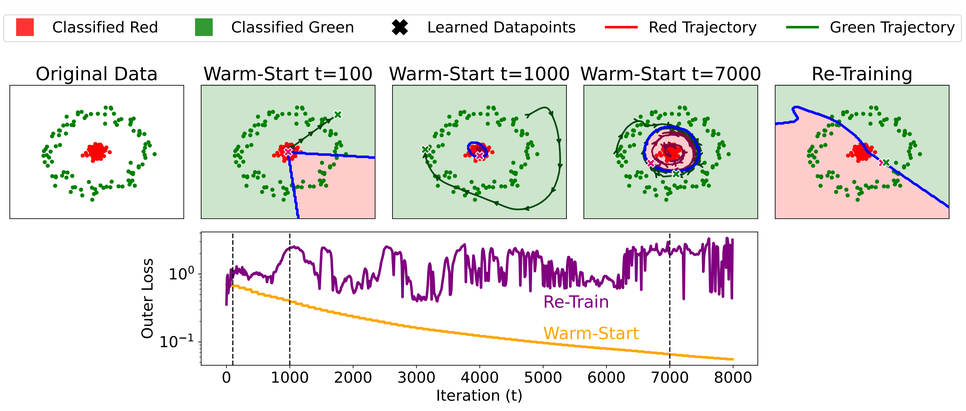
- Assuming F and f are quadratic and we use exact hypergradients, the converged $\mathbf{u}^\star$ minimizes distance to $\mathbf{u}_0$: $\operatorname{argmin}_{\mathbf{u}\in\operatorname{argmin}_{\mathbf{u}} F(\mathbf{u},\mathbf{w}^\star)} \|\mathbf{u} - \mathbf{u}_0\|_2^2$. ($\mathbf{u}_0 = 0$ gives min-norm)
- For strongly-convex f, full warm-start ≡ cold-start
- Under conditions, full warm-start ≡ partial warm-start.

Warm-Start vs Cold-Start Solution Concepts

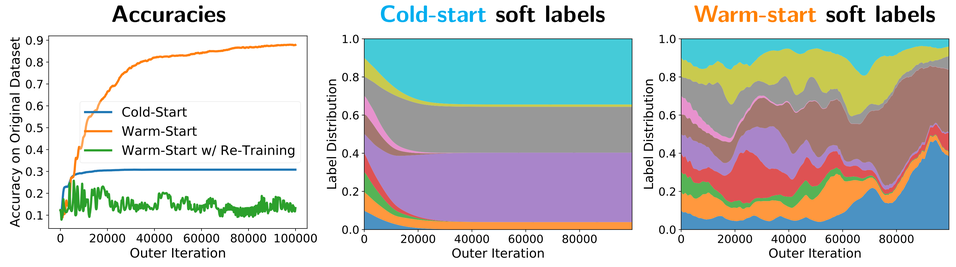


- Dataset distillation for binary classification, with two learned datapoints (outer parameters) adapted jointly with the model weights (inner parameters).
- *Optimistic:* $\mathbf{w}$ achieves the *best outer-objective value*, $\operatorname{argmin}_{\mathbf{w}^*\in\mathcal{S}(\mathbf{u})} F(\mathbf{u}, \mathbf{w})$.
- *Pessimistic:* $\mathbf{w}$ achieves the *worst outer-objective value*, $\operatorname{argmax}_{\mathbf{w}^*\in\mathcal{S}(\mathbf{u})} F(\mathbf{u}, \mathbf{w})$.
- *In practice:* Due to implicit bias of gradient descent, the solution $\mathbf{w}^* \in \mathcal{S}(\mathbf{u})$ we end up at depends on the initialization $\mathbf{w}_0$: **cold-start** is biased towards simple solutions (e.g., min-norm solutions for quadratic f)
- With **warm-start**, the trajectory of outer parameters $\mathbf{u}$ during joint optimization influences the inner parameters $\mathbf{w}$.

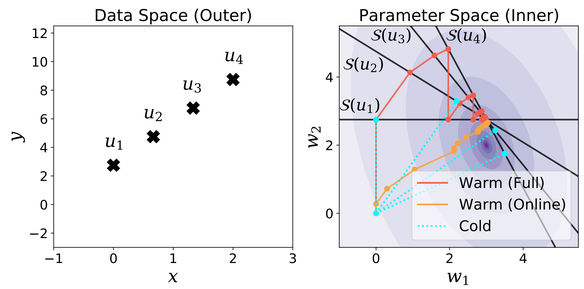
Inner Overparameterization: Dataset Distillation



- Because F is only used to update the outer parameters, one might think that all of the info about F is compressed into $\mathbf{u}$.
- Inner parameters can encode a surprising amount of information about the outer objective, even when the outer parameters are low-dimensional.
- Warm-start BLO yields outer parameters that fail to generalize under re-initialization of the inner problem.

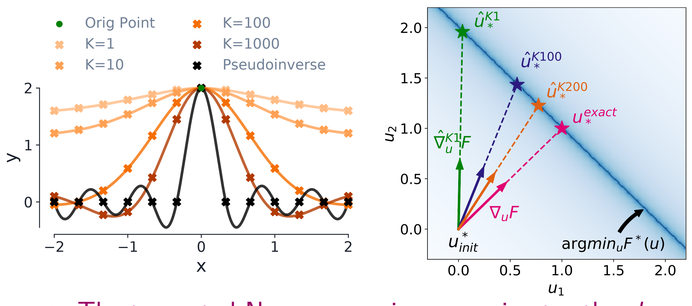


Explaining Warm-Start Memory



- Simplified parameter- and data-space view of warm-start with full inner optimization, warm-start with partial inner optimization, and cold-start optimization.
- Here, we cycle through outer param values $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4\}$
- Cold-start projects from the origin $\mathbf{w}_0$ onto the solution set for the current datapoint, $\mathcal{S}(\mathbf{u})$.
- Full warm-start projects from the current weights $\mathbf{w}_k$.
- If we successively project between solution sets, $\mathbf{w}$ can converge to the intersection of solution sets, so $\mathbf{w}$ can perform well for multiple $\mathbf{u}$ simultaneously.

Implicit Bias from Hypergradient Approximation



- The truncated Neumann series approximates the *damped Hessian inverse*: $\alpha\sum_{j=0}^{K}(\mathbf{I}-\alpha\mathbf{H})^j \approx (\mathbf{H}+\epsilon\mathbf{I})^{-1}$ where $\epsilon = \frac{1}{\alpha K}$.
- The damping prevents the inner optimization from moving far in low-curvature directions.
- **Anti-distillation:** more distilled datapoints than original datapoints. We learn the y-coord of 13 synthetic datapoints such that a regressor trained on them will fit a single original datapoint, at the green dot.
- **Left:** learned datapoints (outer parameters) from different hypergradient approximations: truncated Neumann/diff-through-unrolling with different # steps K
- **Right:** The exact hypergradient leads to the min-norm solution $||\mathbf{u} - \mathbf{u}_0||^2$, while approximate Neumann hypergradients lead to different (valid) outer solutions.