Abstract
Learning to optimize has emerged as a powerful framework for various optimization tasks.
- Current such “meta-optimizers” often learn from the space of continuous optimization algorithms that are point-based and uncertainty-unaware.
- We learn in an extended space of both point-based and population-based optimization algorithms.
- We incorporate the Boltzmann-shaped posterior into meta-loss to guide the search in the algorithmic space and balance the exploitation-exploration trade-off.
- Empirical results over non-convex test functions and the protein docking application demonstrate that this new meta-optimizer outperforms existing competitors.

Methods
- **Updating Rules**: Iterative optimization algorithms, either point-based or population-based, have a common generic expression of update formulas:
  \[ x^{t+1} = x^t + \delta x^t \]
  The update is often a function \( g(\cdot) \) of the historic sample values, objective values, and gradients. For instance: in particle swarm optimization (PSO), we have
  \[ \delta x^t = g(x^t, f(x^t), \nabla f(x^t)) \]
  In our approach, we parameterize the update rule \( g(\cdot) \) through RNN, and introduce **intra- and inter-particle attention mechanisms**:
  \[ g(x) = \text{RNN}(\alpha_{\text{inter}}(\{w^t(x_i^{(t)} | S^t_{\text{in}})\}_{i=1}^{n}), \alpha_{\text{inter}}(\{w^t(x_i^{(t)} | S^t_{\text{in}})\}_{i=1}^{n}), \alpha_{\text{intra}}(\{w^t(x_i^{(t)} | S^t_{\text{in}})\}_{i=1}^{n}) \]
- **Population-based and Point-based Features**: Inspired from both point- and population-based algorithms, we choose the following four features for particle \( i \) at iteration \( t \):
  - **Grad**: \( F(x^t) \)
  - **Momentum**: \( m_i = (1 - \beta)d^t \nabla f(x^t) \)
  - **Velocity**: \( v_i = \alpha \cdot v_i - \delta x^t \)
  - **Attention**: \( \text{softmax} \) for all \( j \) that \( f(x_j^t) < f(x_i^t) \), \( \alpha \) is the hyperparameter and \( d_i = |x_i - x_j| \)
- **Loss Function**: In order to balance the exploitation–exploitation tradeoff, we combine the cumulative regret and the entropy of the posterior over the global optimum:
  \[ f_j(\phi) = \frac{1}{3} \sum_{i \neq j} f(x_i^t) + \lambda \log(p(x_i^t, D_i, X_j^t)), \]
  where the posterior is a Boltzmann distribution \( \beta \):
  \[ p(x_i^t, D_i, X_j^t) \propto \exp(-\beta f(x_i^t)) \]

Test Function Results
- **LOHS outperforms DM_LSTM** [1] and hand-engineered algorithms for non-convex Rastrigin functions:
  \[ f(x) = \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} \cos(2\pi x_i) + a \]

Protein Docking Results
- **Ab initio protein docking** represents a major challenge for optimizing a noisy and costly function in a high-dimensional space [3]. We parameterize the search space as \( \mathbb{R}^{2D} \) as in [3]. The final \( f(x) \) is fully differentiable and the search space is \( x \in \mathbb{R}^{2D} \).
- **LOHS outperforms PSO3 in energy scores for three protein-protein pairs of various difficulty levels.**

References

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