Improving CLIP Training with Bayesian Optimization

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Abstract

Global contrastive learning has gained significant attention for its ability to leverage dataset-wide statistics, offering robust representation learning in multimodal settings such as image-text pairs. This project focuses on optimizing global contrastive loss functions, including stochastic optimization for global contrastive learning (SogCLR) and indvidual SogCLR (iSogCLR) variants, to enhance performance in multimodal self-supervised learning tasks.

Through systematic evaluation and optimization using advanced optimizers such as AdamW and RAdam, we achieve significant improvements over both the benchmark CLIP model and the provided codebase (*SogCLR*). Specifically, our proposed workflow improves ImageNet ACC@1 by **37.6**%, and MSCOCO TR@1 by **23.8**%, MSCOCO IR@1 by **12.8**% compared to the original CLIP model, resulting in an overall **28.3%** improvement in the average score. Furthermore, compared to the provided *SogCLR* implementation, our method achieves **10.3**% improvement in the overall average with substantial improvement in ImageNet ACC@1 by **19.7**% .

This work is publicly available at this GitHub repository.

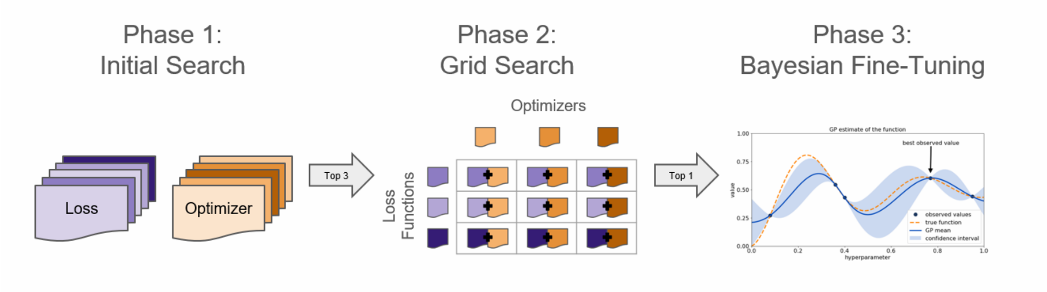
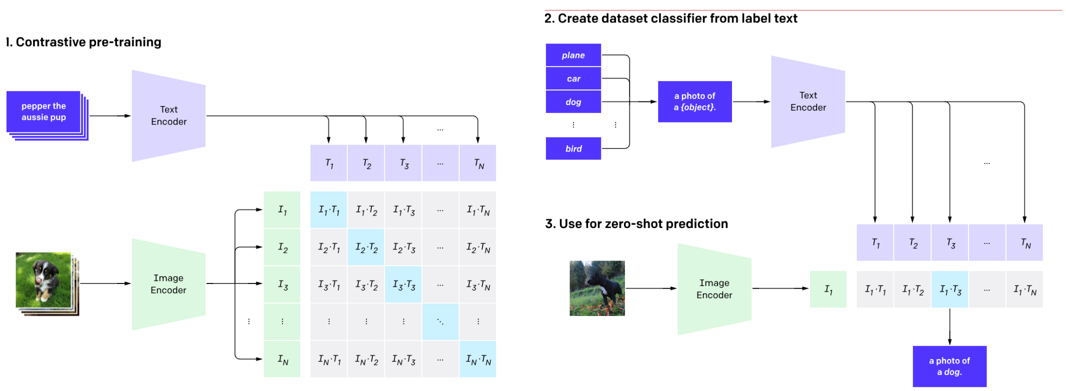


Figure 1: Graphical Abstract.

Contents

1 Introduction

Contrastive learning has revolutionized self-supervised learning by leveraging similarity and dissimilarity comparisons within data to generate high-quality feature representations. In multimodal domains, particularly image-text pairings, contrastive learning has enabled breakthroughs in representation quality, supporting tasks such as zero-shot classification and cross-modal retrieval. CLIP (Contrastive Language-Image Pretraining) [16] exemplifies this paradigm, utilizing local contrastive loss to align visual and textual embeddings within a batch. The architecture for CLIP model is shown in figure 2.



(a) Step 1: Contrastive pre-training. (b) Step 2, 3: Inference.

Figure 2: Overview of the CLIP architecture and workflow, including pretraining and inference stages.

This project advances multimodal self-supervised learning by focusing on global contrastive loss functions, which extend contrastive learning beyond batch-level comparisons to include dataset-wide statistics. These methods offer the potential for more robust feature learning and improved generalization.

In addition to exploring advanced loss functions such as *SogCLR* and *iSogCLR*, we also incorporate state-of-the-art Bayesian optimization techniques to tune hyperparameters.

The objective of this project is to enhance the training of CLIP-like models through the development and evaluation of better algorithms for global contrastive loss optimization.

More specifically, **our contributions in this project are**:

- Explore global loss functions, including state-of-the-art techniques such as *SogCLR* and *iSogCLR*, alongside their optimizations.
- Investigate the effectiveness of Bayesian optimization and advanced optimizers, such as AdamW, RAdam in improving the convergence and performance of these global losses.

The rest of this document is organized as follows: Section 2 gives the necessary background to understand the context of this project including detailed theory about each component of this project. In section 3, we breifly describe the related research work that we build on to make this project successful. In section 4, we clearly define the modeling approach including the evaluation procedure. Finally, section 5 explains in details the experimental setup and the results obtained in the training and evaluation process. We then conclude by comparing our performance with the available benchmarks.

2 Background

2.1 Self-Supervised Learning and Contrastive Learning

Self-Supervised Learning (SSL) has become a foundational paradigm for pre-training deep neural networks, demonstrating effectiveness across a wide range of domains, including Natural Language

Processing (NLP) [14, 4, 10] and Computer Vision (CV) [5, 21, 12]. SSL aims to learn generalizable data representations from unlabelled data, which can then be transferred to various downstream tasks.

Contrastive Learning (CL) has emerged as a simple yet powerful framework within SSL. It aligns representations of "positive" pairs (e.g., augmented views of the same image) while pushing apart "negative" pairs (e.g., augmented views of different images). CL has achieved state-of-the-art results in image and text representation learning [3, 7, 18, 8]. Extending CL to multimodal data, where images and text are treated as different views of the same concept, has enabled models like CLIP [16] to achieve remarkable performance on various visual understanding tasks.

Despite its success, CLIP's reliance on batch-level contrastive loss introduces challenges, such as sensitivity to mini-batch size and slow convergence, especially in large-scale multimodal datasets. These limitations motivate the development of global contrastive loss functions.

2.2 Local and Global Contrastive Loss

The standard CLIP training methodology uses a mini-batch-based contrastive loss. Let $\mathcal{B}$ be a mini-batch of m image-text pairs (x_i, z_i). For each pair, the contrastive loss contrasts the similarity scores between matching pairs (x_i, z_i) and non-matching pairs (x_i, z_j) and (z_i, x_j) within the batch. The local contrastive loss for the mini-batch is computed as:

$$L(w, \tau, \mathcal{B}) = \frac{1}{m} \sum_{(x_i, z_i) \in \mathcal{B}} \log \left(\frac{\exp(h_i(w)^\top e_i(w)/\tau)}{\sum_{z_j \in \mathcal{B}} \exp(h_i(w)^\top e_j(w)/\tau)} \right) + \text{(symmetric term)},$$

where τ is the temperature parameter, and $h_i(w)$ and $e_i(w)$ are the normalized image and text embeddings, respectively.

While effective for small-scale datasets, the local loss's reliance on mini-batch negatives can lead to suboptimal performance on larger datasets. Global Contrastive Loss (GCL) addresses this issue by contrasting embeddings against the entire dataset:

$$L(w, \tau, \mathcal{D}) = \frac{1}{n} \sum_{x_i \in \mathcal{D}} \log \left(\frac{\exp(h_i(w)^\top e_i(w)/\tau)}{\sum_{z_j \neq z_i} \exp(h_i(w)^\top e_j(w)/\tau)} \right) + \text{(symmetric term)},$$

where $\mathcal{D}$ is the full dataset. By leveraging dataset-wide negatives, GCL improves convergence and representation quality.

2.3 SogCLR and iSogCLR

Training models with GCL is computationally expensive for large datasets. To mitigate this, SogCLR [20] introduces a memory-efficient stochastic optimization approach. The key idea is to maintain moving averages of negative pair contributions:

$$\begin{aligned} u_{1,i,t} &= (1-\gamma) u_{1,i,t-1} + \gamma g_1(w_t, x_i, \mathcal{B}_{1t}^-), \\ u_{2,i,t} &= (1-\gamma) u_{2,i,t-1} + \gamma g_2(w_t, z_i, \mathcal{B}_{2t}^-), \end{aligned}$$

where γ is a smoothing parameter, and g_1 and g_2 are contrastive terms computed over mini-batches. The model parameters are updated using:

$$G_t = \frac{1}{m} \sum_{x_i \in \mathcal{B}_t} \frac{\nabla g_1(w_t, x_i, \mathcal{B}_t)}{\varepsilon + u_{1,i,t}} + \frac{1}{m} \sum_{z_i \in \mathcal{B}_t} \frac{\nabla g_2(w_t, z_i, \mathcal{B}_t)}{\varepsilon + u_{2,i,t}}.$$

This approach enables efficient optimization of the global objective without requiring full dataset computations.

iSogCLR [15] extends SogCLR by dynamically optimizing the temperature parameter τ, treating it as a trainable variable. This is achieved through a robust optimization framework:

$$\min_{w, \tau_1, \tau_2} \frac{1}{n} \sum_{x_i \in \mathcal{D}} L_1(w, \tau_{i1}, x_i, \mathcal{D}) + \frac{1}{n} \sum_{z_i \in \mathcal{D}} L_2(w, \tau_{i2}, z_i, \mathcal{D}) + \rho \sum_{i=1}^{n} (\tau_{i1} + \tau_{i2}),$$

where ρ is a regularization parameter. This formulation improves the robustness of learned representations, particularly for imbalanced datasets.

2.4 Datasets and Metrics

This project adheres to fixed datasets and evaluation criteria to ensure consistent and fair evaluation:

Datasets:

- **Training:** A 100k subset of the Conceptual Captions 3M (CC3M) dataset, which contains diverse and noisy image-text pairs derived from web data. It is designed to train models for learning robust image-text alignments.
- **Validation:**
  - **MSCOCO:** A large-scale dataset of high-quality image-text pairs focused on common objects in context, commonly used for image-to-text and text-to-image retrieval tasks.
  - **ImageNet:** A benchmark dataset comprising labeled images across 1,000 categories, used here for evaluating zero-shot image classification.

Metrics: The performance of models is evaluated based on three metrics:

- **Image-to-Text Recall at Rank 1 (IR@1):** Measures the percentage of images whose corresponding text is ranked first in a retrieval task. Higher IR@1 indicates better alignment between image and text embeddings.
- **Text-to-Image Recall at Rank 1 (TR@1):** Measures the percentage of text queries whose corresponding images are ranked first in a retrieval task. Higher TR@1 reflects improved cross-modal retrieval accuracy.
- **Top-1 Accuracy (ACC@1):** For zero-shot classification, ACC@1 computes the proportion of test samples where the predicted class (from image embeddings) matches the ground-truth label. It indicates the model's ability to generalize to unseen classes.

The overall evaluation metric is the average of IR@1, TR@1, and ACC@1, providing a unified measure of retrieval and classification performance.

2.5 Bayesian Optimization for Hyperparameter Tuning

Efficient hyperparameter tuning is crucial for improving model performance, particularly in complex optimization problems like global contrastive loss. Bayesian optimization is a probabilistic model-based approach that optimizes a target function by iteratively constructing a surrogate model. This model predicts the objective's behavior based on prior evaluations, guiding subsequent hyperparameter selections to balance exploration and exploitation [17].

Bayesian optimization employs acquisition functions, such as Expected Improvement (EI) or Upper Confidence Bound (UCB), to determine the next set of hyperparameters to evaluate. Unlike grid or random search, which sample hyperparameters indiscriminately, Bayesian optimization strategically narrows the search space, significantly reducing computation time while improving results. This efficiency has led to its adoption in various machine learning domains espicially large-scale neural network training [17, 2, 9].

In this project, Bayesian optimization is applied to tune critical hyperparameters, such as the learning rate, temperature parameter τ, and optimizer configurations, to enhance the training of CLIP-like models with global contrastive loss.

3 Related Work

Self-supervised learning (SSL) has revolutionized representation learning by leveraging unlabeled data to learn robust features. Contrastive learning, a prominent approach within SSL, trains models by contrasting positive pairs against negative pairs. Early works like SimCLR [3] and MoCo [7] established the foundations of contrastive learning, primarily focusing on single-modality tasks.

Multimodal contrastive learning extends these concepts to multiple data modalities, such as image and text, as demonstrated by CLIP [16]. CLIP optimizes a local contrastive loss over mini-batches, achieving remarkable zero-shot capabilities. However, its reliance on mini-batch statistics limits scalability and convergence for large datasets.

To address these limitations, global contrastive loss functions have been introduced:

- **SogCLR** [20]: Maintains dataset-level statistics to overcome the dependence on mini-batch size.
- **iSogCLR** [15]: Extends SogCLR by incorporating temperature learning and advanced regularization techniques, including DRO mechanisms.
- **Global Objectives**: Other global loss methods explore dataset-wide invariance and variance constraints, such as VICReg [1].

Parallelly, advancements in optimizers like AdamW [13], NovoGrad [6], and RAdam [11] have improved optimization dynamics for large-scale learning tasks. This project builds upon these developments by systematically evaluating global contrastive losses and their interaction with advanced optimizers.

4 Modeling

The provided modeling framework is designed to flexibly support training and evaluation of multimodal contrastive learning models, with a specific focus on optimizing loss functions and hyperparameters. At its core, the pipeline implements a CLIP-like architecture, combining a pretrained image encoder and text encoder to learn aligned representations for images and text.

4.1 Modular Design for Loss Functions and Optimizers

The codebase is refactored to enable seamless experimentation with various global contrastive loss functions, including *SogCLR*, *iSogCLR*, and their variants. Each loss function is integrated as a modular component, allowing dynamic configuration based on the desired training objective. Similarly, the optimizer setup supports a wide range of algorithms such as AdamW, Novograd, and their fused counterparts, ensuring compatibility with diverse optimization strategies.

4.2 Model Architecture

The architecture includes:

- **Image Encoder:** A ResNet-50 backbone from the `timm` library, pretrained on ImageNet, processes image inputs.
- **Text Encoder:** A DistilBERT model from the `huggingface` library, pretrained on BookCorpus and Wikipedia, encodes text inputs.
- **Projection Layers:** Linear layers project image and text embeddings into a shared latent space for contrastive learning.

4.3 Training and Evaluation Pipeline

The pipeline supports both training and evaluation workflows:

- **Training:** The framework implements distributed training with support for gradient scaling (for mixed precision) and dynamic learning rate scheduling. Loss gradients are backpropagated and parameters updated based on the selected loss function and optimizer.
- **Evaluation:** Validation includes retrieval tasks (Image-to-Text and Text-to-Image) and zero-shot classification, using pre-defined datasets such as MSCOCO and ImageNet. Based on an objective score evaluated on the validation sets, the best model is selected.

  The objective value is described in 1:

$$\text{Objective Value} = \frac{1}{3}(\text{IR@1} + \text{TR@1} + \text{ACC@1}), \tag{1}$$

where:

- IR@1: Image-to-Text Recall at Rank 1, measuring the proportion of images whose corresponding text is ranked first.
- TR@1: Text-to-Image Recall at Rank 1, quantifying the percentage of text queries whose matching images are ranked first.
- ACC@1: Top-1 Accuracy, indicating the proportion of correct classifications for zero-shot classification tasks.

4.4 Customization for Experimentation

The framework is designed with high flexibility:

- **Loss Function Optimization:** Parameters specific to each loss function, such as temperature τ or regularization terms, are tunable.
- **Optimizer Configurations:** A wide range of optimizer settings can be tested, enabling thorough exploration of optimization dynamics.
- **Checkpointing and Resuming:** Training states can be saved and resumed, ensuring efficient experimentation.

This modular and extensible design facilitates systematic exploration of loss functions, optimizers, and hyperparameters, aligning with the project's goal of optimizing global contrastive learning frameworks.

5 Experiments & Results

This section describes the experimental setup, evaluation protocol, and results for optimizing global contrastive loss functions across three phases. Each phase incrementally narrows the hyperparameter search space, focusing on identifying and tuning the best-performing configurations.

5.1 Experimental Setup

The experiments are conducted in three phases:

1. **Phase 1: Initial Search.** A Bayesian search explores combinations of loss functions and optimizers over a wide search space. Experiments run for 10 epochs using 20% of the training data.
2. **Phase 2: Grid Search.** Top combinations identified in Phase 1 are trained on the full dataset for 15 epochs. A grid search refines the hyperparameter space for selected loss functions and optimizers.
3. **Phase 3: Fine-Tuning.** The best-performing configuration from Phase 2 undergoes a comprehensive hyperparameter search and is trained for 30 epochs with the full training dataset.

5.2 Results

5.2.1 Phase 1: Initial Search

In this phase, we explored 10 optimizers and 3 loss functions, as shown in the search space below:

- **Loss Functions:** SogCLR, iSogCLR_New, iSogCLR_New_v2.
- **Optimizers:** Adam, AdamW, RAdam, NovoGrad, FusedAdam, FusedLAMB, FusedNovoGrad, RMSProp, Momentum, NVNovoGrad.

The primary goal was to identify sensitivity of the objective metric to different combinations of loss functions and optimizers. The results are visualized in Figure 3 and Figure 4.

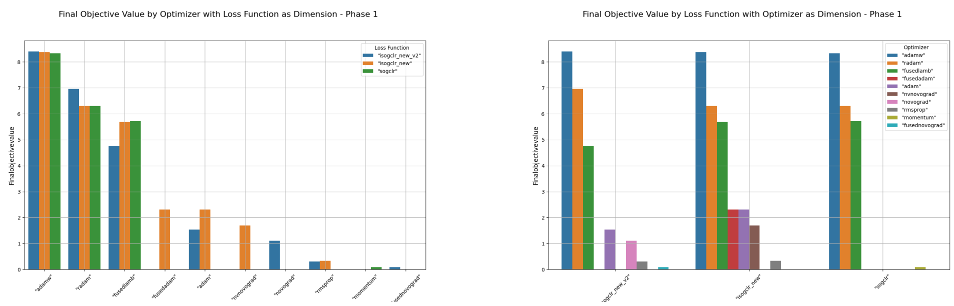


Figure 3: (Left) Validation objective values by optimizer, with loss function as dimension. (Right) Validation objective values by loss function, with optimizer as dimension (Phase 1).

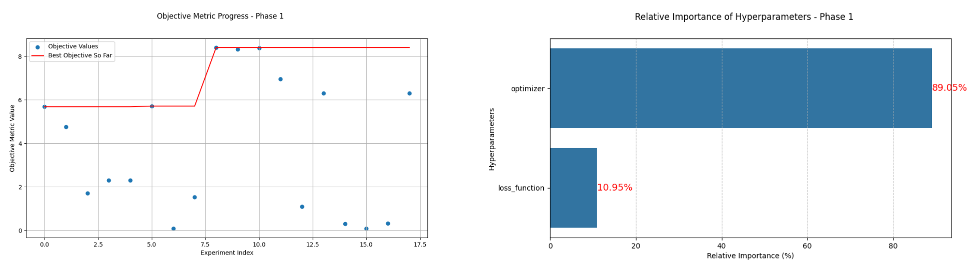


Figure 4: (Left) Progression of objective metric. (Right) Relative importance of hyperparameters (Phase 1).

5.2.2 Phase 2: Grid Search

Based on insights from Phase 1, we selected the top 3 optimizers (AdamW, RAdam, FusedLAMB) and 3 loss functions (SogCLR, iSogCLR_New, iSogCLR_New_v2) for grid search on the full dataset. The search space was refined to focus on specific hyperparameters relevant to these configurations.

The optimizers tested included AdamW, RAdam, FusedLAMB, each offering unique advantages. AdamW [13], known for its weight decay regularization, is widely used for stable training in deep learning models. RAdam [11], or Rectified Adam, enhances stability during training by rectifying variance in adaptive learning rates. FusedLAMB [19] is optimized for GPU efficiency, offering faster computations with lower memory usage.

The results for this phase are visualized in Figure 5 and Figure 6, while Table 1 summarizes the important hyperparameters used for both phase 1 and 2.

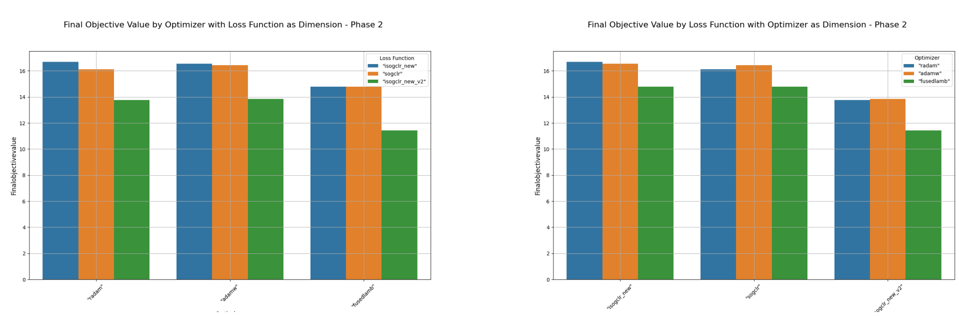


Figure 5: (Left) Validation objective values by optimizer, with loss function as dimension. (Right) Validation objective values by loss function, with optimizer as dimension (Phase 2).

5.2.3 Phase 3: Fine-Tuning

In the final phase, we trained the best-performing configuration (`iSogCLR_New` with `RAdam`) on the full dataset for 30 epochs. The hyperparameters tuned in this phase included learning rate, weight

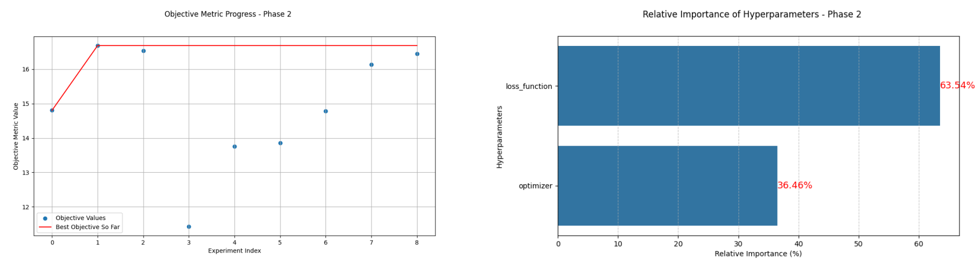


Figure 6: (Left) Progression of objective metric. (Right) Relative importance of hyperparameters (Phase 2).

Parameter	Value	Description
`embed_dim`	256	Dimensionality of the embedding space for image and text representations.
`lr`	0.0002	Learning rate for the optimizer.
`warmup_epochs`	5	Number of warmup epochs where the learning rate gradually increases.
`cooldown_epochs`	0	Number of cooldown epochs after training where learning rate gradually decreases.
`batch_size_train`	128	Batch size used during training.
`sogclr_gamma`	0.8	Momentum coefficient for the SogCLR loss function.
`rho_I`	8.0	Regularization coefficient for image embeddings in iSogCLR_New.
`rho_T`	8.0	Regularization coefficient for text embeddings in iSogCLR_New.
`eta_init`	0.001	Initial step size for specific loss function updates.
`tau_init`	0.01	Initial temperature for contrastive loss.
`personalized_tau`	0	Boolean indicating whether to use personalized temperatures for each sample.
`learnable_temp`	0	Boolean indicating whether the temperature parameter is learnable.

Table 1: Important hyperparameters and their descriptions for Phases 1 and 2.

decay, and loss-specific parameters such as the temperature. The progression of the objective metric is shown in Figure 7. The winning parameters are summarized in table 2.

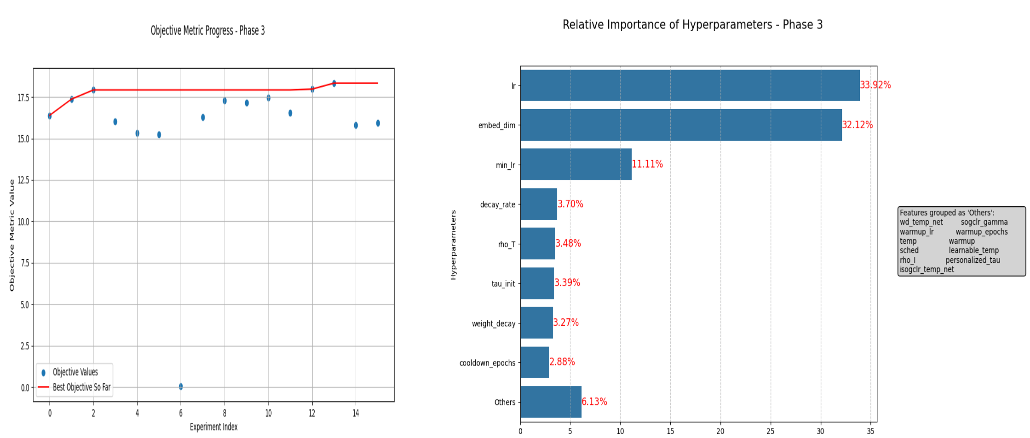


Figure 7: (Left) Progression of objective metric. (Right) Relative importance of hyperparameters (Phase 3).

Hyperparameter	Value	Range	Description
`lr`	1.64e-4	$[1e-4, 1e-2]$	Learning rate for the RAdam optimizer.
`weight_decay`	3.73e-4	$[1e-6, 1e-2]$	Weight decay for the RAdam optimizer.
`embed_dim`	512	$\{64, 128, 256, 512, 1024\}$	Dimensionality of the shared image-text embedding space.
`sogclr_gamma`	0.966	$[0.5, 1.0]$	Momentum coefficient for updating moving averages in the SogCLR loss function.
`rho_I`	9.96	$[1, 10]$	Regularization coefficient for image embeddings in *iSogCLR_New*.
`rho_T`	7.47	$[1, 10]$	Regularization coefficient for text embeddings in *iSogCLR_New*.
`tau_init`	0.01	$[0.01, 0.1]$	Initial temperature for the contrastive loss.
`temp`	5.85e-2	$[0.01, 0.1]$	Initial global temperature parameter for contrastive loss.
`wd_temp_net`	5.85e-6	$[1e-6, 1e-2]$	Weight decay for the temperature network parameters.
`decay_rate`	0.5679	$[0.5, 1.0]$	Decay rate for the learning rate scheduler.
`min_lr`	1.0e-5	$[1e-7, 1e-5]$	Minimum learning rate during learning rate scheduling.
`cooldown_epochs`	1	$[0, 5]$	Number of cooldown epochs for gradual learning rate reduction.
`warmup_epochs`	5	$[0, 5]$	Number of warmup epochs where the learning rate gradually increases.
`warmup_lr`	1.0e-3	$[1e-5, 1e-3]$	Initial learning rate during warmup phase.
`sched`	`tanh`	$\{\text{cosine}, \text{tanh}\}$	Learning rate scheduler type.

Table 2: Tuned hyperparameters from Phase 3.

5.2.4 Best Training Job Analysis

In figure 8, we show the learning progress for the best-performing job (its parameters are tabulated in table 2). It can be noticed the rapid progress achieved in the first 23 epochs (best epoch) before the performance almost saturates. This suggests using early stopping in the future to reduce the training cost.

5.3 Discussion

From Phase 1 experiments, the Bayesian search efficiently explored the search space giving us important insight about the critical role of the optimizer (89%) over the loss function (11%). Phase 2 helped giving a direction for which configuration to fully tune. Finally, Phase 3 results shown in figure 7 demonstrates the relative importance played by each dimension to make the Bayesian search select the next experiment.

Of the hyperparameters documented in Table 3, the learning rate (lr), embedding dimension (embed_dim), and minimum learning rate (min_lr) had the most significant impact on model performance. The learning rate is critical for achieving a balance between fast convergence and stable training. A higher learning rate could accelerate model convergence but risked overshooting optimal solutions, especially when optimizing the global contrastive losses used in this project. Conversely, a lower learning rate ensures gradual progress but could prolong training. The final value allowed the model to

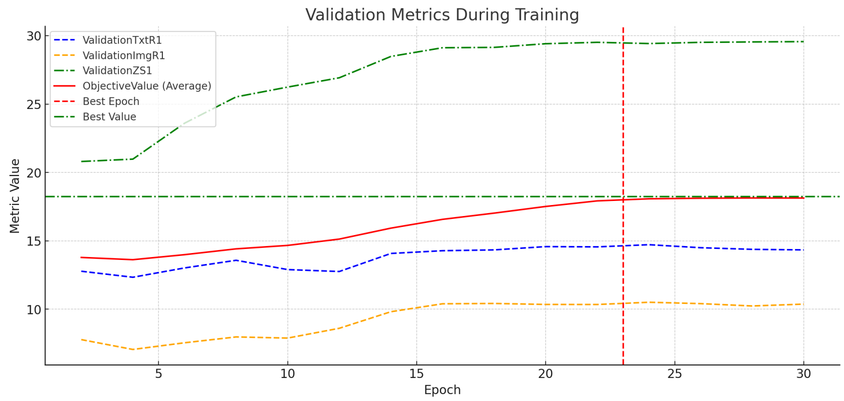


Figure 8: Validation metrics progression for the best-performing configuration during Phase 3 fine-tuning.

leverage the strengths of RAdam, enabling consistent improvements across epochs while maintaining stability of dataset-wide statistics.

The chosen embedding dimension enhanced the representational capacity of the model, enabling it to capture nuanced multimodal alignments between image and text embeddings. Larger embeddings, while computationally expensive, proved essential for achieving superior results in retrieval and zero-shot classification tasks.

Similarly, the minimum learning rate provided a safety net during the later stages of training, ensuring that learning rate decay did not hinder fine-tuning. This allowed the model to refine embeddings while maintaining performance consistency.

6 Conclusion

Our experiments demonstrate that both *SogCLR* and *iSogCLR_New* loss functions significantly outperform the benchmark CLIP model across key metrics on the MSCOCO and ImageNet datasets. Notably, *iSogCLR_New* achieves the highest average score of 18.25, representing a substantial improvement of 28.3% over the CLIP baseline and 10.3% over the SogCLR model. These results affirm the effectiveness of optimizing global contrastive loss functions combined with advanced hyperparameter tuning and structured training workflows.

The table below summarizes the performance gains achieved by our methods. The best results for each metric are bolded, and percentage improvements relative to the CLIP baseline are shown in parentheses for clarity.

Method	MSCOCO TR@1	MSCOCO IR@1	ImageNet ACC@1	Average
CLIP (Benchmark)	12.00	9.32	21.35	14.22
SogCLR (Provided Codebase)	14.38 (+19.8%)	**10.73** (+15.1%)	24.54 (+15.0%)	16.55 (+16.4%)
iSogCLR_New (Ours)	**14.86** (+23.8%)	10.51 (+12.8%)	**29.37** (+37.6%)	**18.25** (+28.3%)

Table 3: Comparison of different benchmarks on validation datasets. Improvements relative to CLIP are shown in parentheses, and the best results are bolded.

These findings underscore the advancements achieved by our work, particularly with the *iSogCLR_New* loss function, which consistently outperforms both the baseline and existing methods. The superior performance across all metrics demonstrates its potential for enabling scalable and efficient multimodal self-supervised learning, setting a new standard for future developments in the field.

Team Contributions

This section outlines the contributions of each team member to the project.

Omar Khater

- Initiated the project by interacting with the provided codebase.
- Planned the work strategy and outlined a systematic experimental approach.
- Project Report.
- Training for all phases.
- Results analysis.

Michael Norman

- Researched ways to increase speed of model training and evaluation functions.
- Researched and set efficient hyperparameter ranges for fine tuning.
- Debugged training code to allow for hyperparameters to be set and run successfully.
- Created project presentation.
- Reproduced training and evaluation results for final model.

Declaration

We acknowledge that generative AI technologies, including OpenAI's ChatGPT, were utilized to assist in drafting this report. The AI tools provided support in organizing ideas, structuring sections, and refining the language of the document.

The authors, Omar Khater and Michael Norman, have thoroughly reviewed the report and confirm its content. We take full responsibility for the ideas, analyses, and conclusions presented in this report.

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