

Best of Both Worlds: Multimodal Contrastive Learning with Tabular and Imaging Data

Image Modality + Tabular Modality (more than 120 clinical features)

Paper: <https://arxiv.org/pdf/2303.14080.pdf> (CVPR)

Code: <https://github.com/paulhager/MMCL-Tabular-Imaging>

1. Data augmentation for both imaging and tabular data
2. Augmented Images -> Image Encoder (ResNet50) -> Image Projection Head (MLP) -> Normalization
3. Augmented Tabular Data -> Tabular Encoder (MLP) -> Tabular Projection Head (A Fully Connected Layer) -> Normalization
4. Cosine Similarity + SoftMax + Negative Log Loss for each modality loss
5. Understand the importance of each tabular
 - a. Integrated Gradients
6. Incorporated Labels into the Tabular feature
7. Datasets:
 - a. Cardiac MR images + Clinical Information (UK Biobank)
 - b. Data Visual Marketing dataset
8. Results:
 - a. Better accuracy in the downstream linear probing tasks in both datasets
 - b. Better performance under imbalanced datasets such as rare disease
 - c. Morphometric features such as size and shape are more critical tabular features
 - d. Adding a label as a tabular feature boosts the performance of supervised contrastive learning

ContIG: Self-supervised Multimodal Contrastive Learning for Medical Imaging with Genetics

Imaging + Several Genetic Modalities

Paper:

https://openaccess.thecvf.com/content/CVPR2022/papers/Taleb_ContIG_Self-Supervised_Multimodal_Contrastive_Learning_for_Medical_Imaging_With_Genetics_CVPR_2022_paper.pdf (CVPR)

Code: <https://github.com/HealthML/ContIG>

1. Encoder (ResNet50) for images and distinct encoder (MLPs) for each genetic modality, plus nonlinear MLP projection heads
2. Cosine Similarity + SoftMax + Negative Log Loss for each modality loss
3. Generalized Multimodal Contrastive Loss: Summation of the pairwise contrastive loss between images and each genetic modality
4. Genetic Feature Explanation:
 - a. Integrated Gradients
5. Datasets: UK Biobank
6. Results:
 - a. Evaluate the quality of embeddings by fine-tuning for four downstream prediction tasks
 - b. Genome-wide Association Study

Matching single cells across modalities with contrastive learning and optimal transport
Raw Single Cell Data from modalities A & B: Cell Matching for Different Single Cell Data Types

Paper: <https://academic.oup.com/bib/article/24/3/bbad130/7147026> (Briefings in Bioinformatics)

Code: <https://github.com/AI4SCR/MatchCLOT>

1. Preprocessing:
 - a. Reduce Dimensions: Latent Semantic Indexing
 - b. Batch Effects Correction: Harmony
2. Training:
 - a. Encoders: Two MLPs
 - b. InfoNCE Loss
3. Cell Matching:
 - a. Optimal Transport + Match with Batch Label Information
4. Datasets: CITE-seq and 10X Multiome Data
 - a. ATAC -> GEX & GEX -> ATAC
 - b. GEX -> ADT & ADT -> GEX
5. Outperform state-of-the-art modality matching methods

Contrastive learning enables rapid mapping to multimodal single-cell atlas of multimillion-scale

Cells

Paper: <https://www.nature.com/articles/s42256-022-00518-z#Abs1> (Nature Machine Intelligence)

Code: <https://github.com/melobio/Concerto-reproducibility>

1. Self-distillation asymmetric network structure (asymmetric teacher-student network structure) + Contrastive Learning -> Generate cell embeddings from Gene Index and Count Value
 - a. Student Network: Count Value -> MLP -> Dropout -> Projection -> Student View Embedding
 - b. Teacher Network: Gene Index + Count Value -> Attention -> Dropout -> Projection -> Teacher View Embedding
2. Datasets:
 - a. Human Peripheral Blood Mononuclear Cell Dataset: PBMC45k
3. Results:
 - a. Contrastively learned embeddings notably boost the performance of cell classification
 - b. Contrastively learned embeddings have better unsupervised clustering over the multimodal dataset

Multimodal contrastive representation learning for drug-target binding affinity prediction

String and Graph Modalities

Paper:

https://www.sciencedirect.com/science/article/pii/S1046202323001871?casa_token=WHnjUMQID2QAAAAA:qKcBrCaRzvZNVpVkdFEj3m3X9RkBESmTkaC4l0_scaiplrK7AyEMTkaGZLARgKHQsiE8sqExqA (Methods)

Code: <https://github.com/bestdoubleLin/FMDTA>

1. Feature extraction of drug structure and target structure:
 - a. String Modality -> Position Encoding -> Transformer Encoder
 - b. Graph Modality -> GNN
 - c. Contrastive Learning
2. DTA Prediction
3. Datasets: Davis & KIBA Datasets
4. Results:
 - a. Compared to string-based models and graph-based models, achieving lower MSE, higher CI and R2

MMCL-CDR: Enhancing Cancer Drug Response Prediction with Multi-Omics and Morphology Images Contrastive Representation Learning

Copy Number Variation, Gene Expression, Morphology Images of Cell Lines, and Chemical Structure of Drugs

Paper:

<https://academic.oup.com/bioinformatics/advance-article/doi/10.1093/bioinformatics/btad734/7467055> (Bioinformatics)

Code: <https://github.com/catly/MMCL-CDR>

1. Multimodal representation for cancer cell lines:
 - a. RNA-seq: encoder -> projection
 - b. Copy Number Variation: encoder -> projection
 - c. Morphology Image: CNN -> projection
 - d. Contrastive Learning between morphology image and combined omic representation to get cell representation
2. Drug molecular graph representation:
 - a. Molecular Graph: GCN -> Max Pooling -> Drug Representation
3. Final MLPs for predicting cancer drug responses
 - a. Binary Classification: Sensitive vs. Resistant
 - b. Binary Cross Entropy Loss
4. Datasets: GDSC, PubChem, and DMSZ
5. Results:
 - a. Better AUC and AUPRC comparing to other baselines