Contrastive Pre-Training and Multiple Instance Learning for Predicting Tumor Microsatellite Instability

Ronald Nap, Mohammed Aburidi, and Roummel Marcia

University of California, Merced, CA, USA

July 15-19, 2024

This talk

Project goal: Predict tumor Microsatellite Instability from Whole Slide Images using Contrastive Learning and Multiple Instance Learning.

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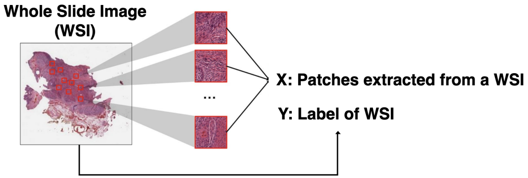
Let

- $\mathbf{X} = \{x_i\}_{i=1}^{N}$: A set of N unlabeled patches extracted from a WSI.
- $\mathbf{Y} = \{y_j\}_{j=1}^{K}$: The set of K true WSI labels corresponding to different MSI statuses in a WSI.



Our approach

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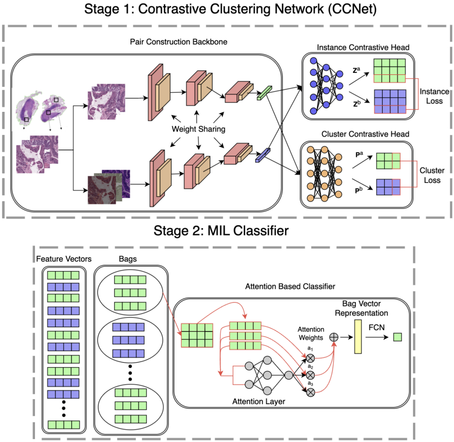

1. Representation Learning with Contrastive Learning

Data Pair Creation:

Data pairs are generated for self-supervised representation learning. These pairs are created by applying various augmentations to the original image, resulting in two transformed versions, $\tilde{\mathbf{X}}^a$ and $\tilde{\mathbf{X}}^b$.

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The following augmentations are applied:

- Random cropping
- Color jittering
- Grayscale transformation
- Horizontal flipping
- Normalization

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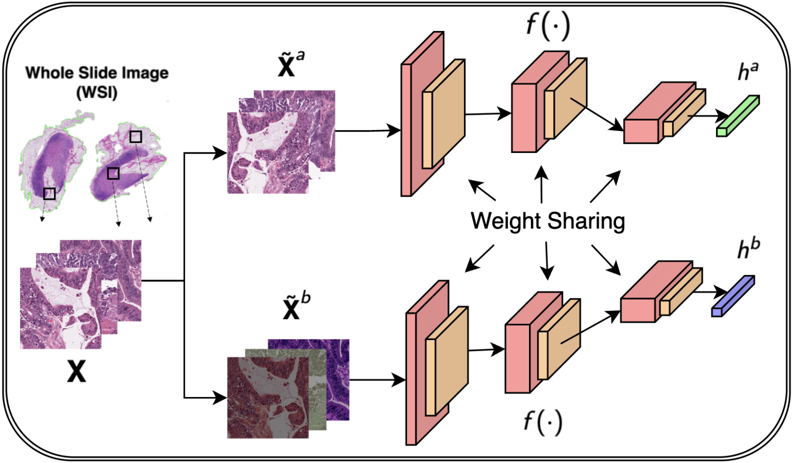

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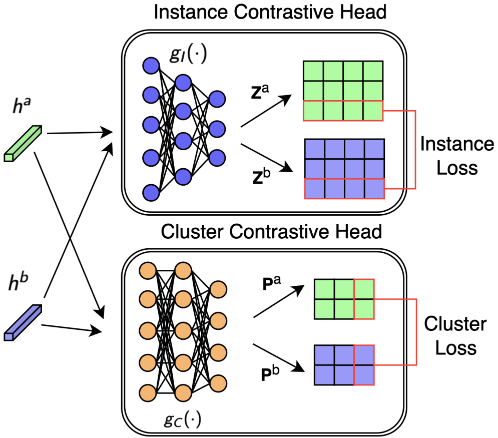

Instance-Level Loss

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$$\mathcal{L}_I = -\sum_{i=1}^{N} \log \frac{\exp(s(z_i^a, z_i^b)/\tau_I)}{\sum_{j=1}^{N} \exp(s(z_i^a, z_j^a)/\tau_I) + \exp(s(z_i^a, z_j^b)/\tau_I)} \quad (1)$$

where $s(\mathbf{u}, \mathbf{v}) = \frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\| \|\mathbf{v}\|}$ is the cosine similarity.

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Overall Loss Function

$$\mathcal{L} = \mathcal{L}_I + \mathcal{L}_C \tag{3}$$

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- Apply augmentations to create pairs of transformed patches.
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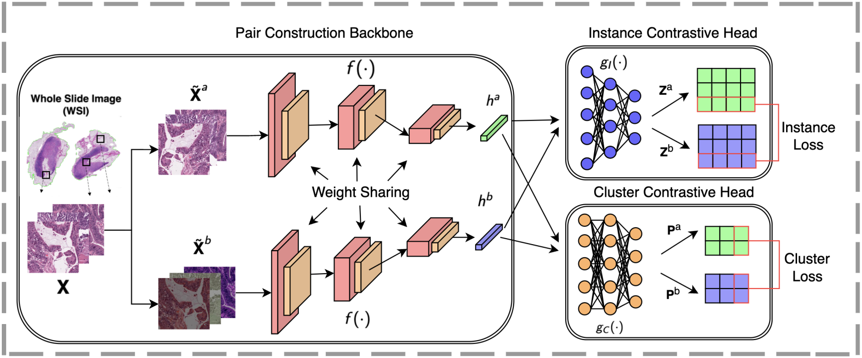
Stage 1: Contrastive Clustering Network (CCNet)



Multiple Instance Learning (MIL)

- MIL is a form of **weakly supervised learning.**
- Suited for scenarios with **uncertainty in labeling** individual data points $\{x_1, \ldots, x_K\}$.
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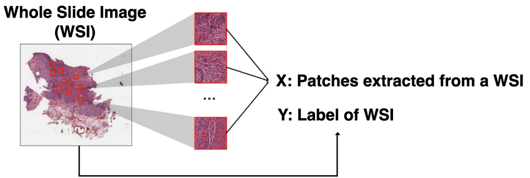
Context: Whole Slide Image (WSI) Analysis

- Treats each WSI as a collection of instances (patches).
- Effective due to the complexities and expansiveness of WSIs.
- Focus on **combined characteristics** of patches.



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$$a_k = \frac{\exp\{\mathbf{W}^\top(\tanh(\mathbf{V}\mathbf{z}_k) \odot \mathrm{sigm}(\mathbf{U}\mathbf{z}_k))\}}{\sum_{j=1}^{N} \exp\{\mathbf{W}^\top(\tanh(\mathbf{V}\mathbf{z}_j) \odot \mathrm{sigm}(\mathbf{U}\mathbf{z}_j))\}} \tag{4}$$

where sigm$(\cdot)$ is the sigmoid function, and $\odot$ is the element-wise product, N is the number of the embedded instance vectors in a bag.

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$$\mu = \frac{1}{N} \sum_{k=1}^{N} a_k \mathbf{z}_k \tag{5}$$

The overall bag representation is computed by the weighted mean μ of these instance embeddings as shown above.

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    - δ - Smoothness parameter ensuring differentiability.
  - Smooth SVM Loss for bag x_j is defined as:

$$l(y_j, f(x_j), \delta) = \begin{cases} \frac{1}{N}\sum_{i=1}^{N} \frac{1}{2\delta}\xi_i^2 & \text{if } \xi_i \leq \delta \\ \frac{1}{N}\sum_{i=1}^{N}(\xi_i - \frac{\delta}{2}) & \text{otherwise} \end{cases}$$

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  - We found that promoting uniform attention within each bag helped prevent overfitting to a few negative instances.

2. Multiple Instance Learning

Overall Workflow:

- Extract patches from WSIs.
- Learn instance-level features using Stage 1 (CCNet).
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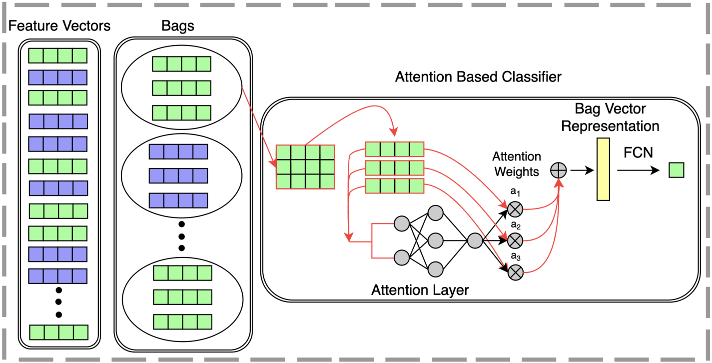
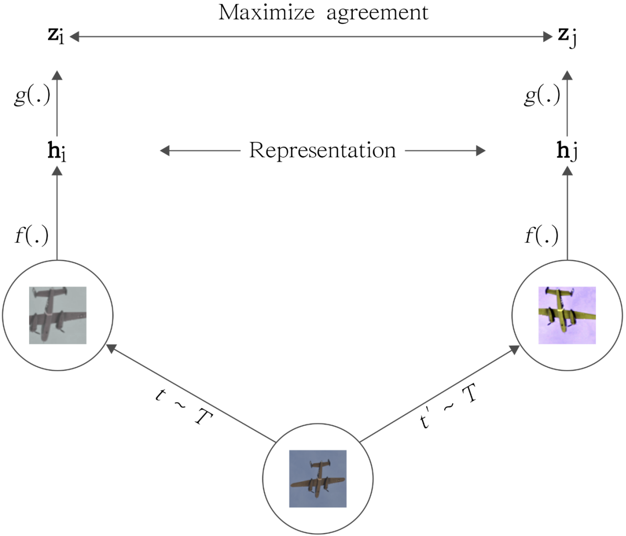
Stage 2: MIL Classifier



3. Numerical results: SimCLR

Contrary to our feature extractor (CCNet), SimCLR only utilizes an instance-level projection head for training.



3. Numerical results: Datasets

Dataset:

- We utilize two image datasets obtained from The Cancer Genome Atlas (TCGA) cohort:
  - The **Colorectal Cancer (CRC) dataset** was utilized for comparative analysis.
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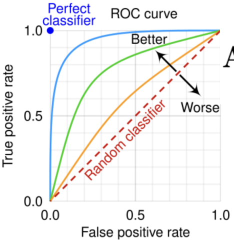
Evaluation:

- We partitioned the training data into 5-folds for cross-validation and reserved the testing split for final validation.

Dataset	Label	# of WSIs		# of Patches		# of Bags	
		Train	Test	Train	Test	Train	Test
CRC	MSI	39	26	46,704	29,335	1850	1122
	MSS	221	74	46,704	70,569	1757	2787
STAD	MSI	35	25	50,285	27,904	N/A	N/A
	MSS	150	74	50,285	90,104	N/A	N/A

3. Numerical results: Evaluation metrics

Area Under the Receiver Operating Characteristic (AUROC)



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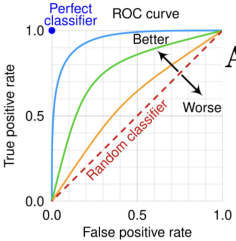

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F1 Score (F1)

True positive (TP)	**False negative (FN)**
False positive (FP)	**True negative (TN)**

$$F1 = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

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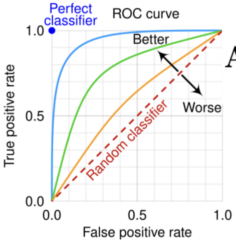

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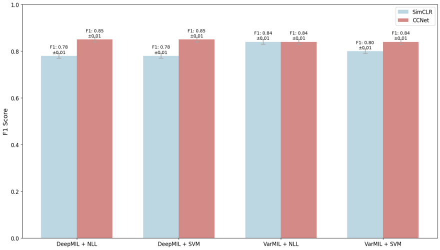
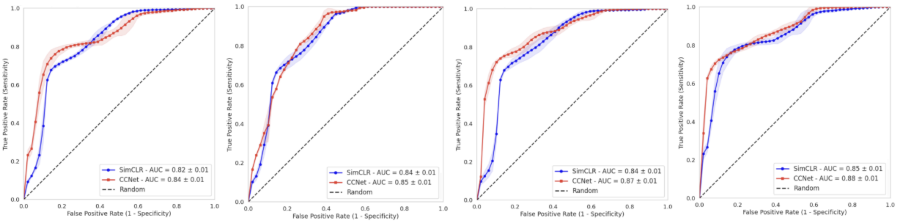
Both measures values between 0 and 1 with higher values indicating better results.

3. Numerical results: CRC Dataset

- To ensure a comprehensive evaluation, we compute the mean and standard deviation of AUROC and F1 scores across five folds.
- We compare the performance of SimCLR with our CCNet extractor.
- We evaluate the efficacy of SVM loss compared to the conventional Negative Log-Likelihood (NLL) loss.
- We employ two attention-based MIL classifiers, DeepMIL and VarMIL, and assess the performance of each model configuration.





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Key Findings:

- CCNet, achieved better AUROC and F1 scores than SimCLR, demonstrating effective feature extraction.

Extractor	Classifier	Loss	AUROC	F1
ResNet18	DeepMIL	NLL	0.58 ± 0.01	0.67 ± 0.01
		SVM	0.58 ± 0.01	0.69 ± 0.01
	VarMIL	NLL	0.59 ± 0.01	0.69 ± 0.01
		SVM	0.59 ± 0.01	0.69 ± 0.01
SimCLR	DeepMIL	NLL	0.81 ± 0.01	0.82 ± 0.01
		SVM	0.82 ± 0.01	0.81 ± 0.01
	VarMIL	NLL	0.78 ± 0.01	0.82 ± 0.01
		SVM	0.81 ± 0.01	0.81 ± 0.01
CCNet	DeepMIL	NLL	0.81 ± 0.01	0.81 ± 0.01
		SVM	0.83 ± 0.01	0.82 ± 0.01
	VarMIL	NLL	0.81 ± 0.01	0.83 ± 0.01
		SVM	0.83 ± 0.01	0.81 ± 0.01

4. Summary

1. Proposed a framework for predicting tumor Microsatellite Instability from Whole Slide Images.

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Thank You!