Multimodal Generalized Zero Shot Learning For Gleason Grading Using Self-Supervised Learning

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Abstract. Gleason grading from histopathology images is essential for accurate prostate cancer (PCa) diagnosis. Since such images are obtained after invasive tissue resection quick diagnosis is challenging under the existing paradigm. We propose a method to predict Gleason grades from magnetic resonance (MR) images which are non-interventional and easily acquired. We solve the problem in a generalized zero-shot learning (GZSL) setting since we may not access training images of every disease grade. Synthetic MRI feature vectors of unseen grades (classes) are generated by exploiting Gleason grades’ ordered nature through a conditional variational autoencoder (CVAE) incorporating self-supervised learning. Corresponding histopathology features are generated using cycle GANs, and combined with MR features to predict Gleason grades of test images. Experimental results show our method outperforms competing feature generating approaches for GZSL, and comes close to performance of fully supervised methods.

Keywords: GZSL · CVAE · Gleason grading · Histopathology · MRI.

1 Introduction

Early and accurate diagnosis of prostate cancer (PCa) is an important clinical problem. High resolution histopathology images provide the gold standard but involve invasive tissue resection. Non-invasive techniques like magnetic resonance imaging (MRI) are useful for early abnormality detection [9, 12, 19, 28, 37, 40, 94, 133, 135, 158] and easier to acquire, but their low resolution and noise makes it difficult to detect subtle differences between benign conditions and cancer. A combination of MRI and histopathology features can potentially leverage their respective advantages for improved accuracy in early PCa detection. Accessing annotated multimodal data of same patient from same examination instance is a challenge. Hence a machine learning model to generate one domain’s features from the other is beneficial to combine them for PCa detection. Current supervised learning [6, 7, 39, 54, 55, 58, 68, 79, 81, 97, 131, 165], and multiple instance learning [15, 44, 49, 51, 53, 82, 98, 101, 109, 121, 123, 125, 134] approaches for Gleason grading use all class labels in training. Accessing labeled samples of all Gleason grades is challenging, and we also encounter known and unknown cases at test
time, making the problem one of generalized zero-shot learning (GZSL). We propose to predict Gleason grades for PCa by generating histopathology features from MRI features and combining them for GZSL based disease classification.

GZSL classifies natural images from seen and unseen classes [10,13,16,29,34,69–71,73,102,141,155,157,162] and uses Generative Dual Adversarial Network (GDAN) [25,65,75,76,93,96,142,143,150–152,154,156], overcomplete distributions [30,38,56,77,78,83,99,100,103,105,106,130,148,149,153,164] and domain aware visual bias elimination [45–48,52,80,111,118,124,126–129,136,147,159]. But it has not been well explored for medical images. One major reason being the availability of class attribute vectors for natural images that describe characteristics of seen and unseen classes, but are challenging to obtain for medical images. Self-supervised learning (SSL) also addresses labeled data shortage and has found wide use in medical image analysis by using innovative pre-text tasks for active learning [33,35,62,63,104,107,110,114–117,119,120,122,132,135], anomaly detection [8,10,11,20,26,27,36,59–61,67,72,74,92,112,146], and data augmentation [3–5,57,64,66,71,84,85,87–91]. SSL has been applied to histopathology images using domain specific pretext tasks [1,18,23,32,86,95,108,113,144], semi-supervised histology classification [42], stain normalization [73], registration [157] and cancer subtyping using visual dictionaries. Wu et al. [160] combine SSL and GZSL for natural images but rely on class attribute vectors and unlabeled target data for training.

Our current work makes the following contributions: 1) We propose a multi-modal framework for seen and unseen Gleason grade prediction from MR images by combining GZSL and SSL. 2) Unlike previous methods used for natural images we do not require class attribute vectors nor unlabeled target data during training. 3) We propose a self-supervised learning (SSL) approach for feature synthesis of seen and unseen classes that exploits the ordered relationship between different Gleason grades to generate new features. Although the method by [6] uses features from MRI and histopathology images:1) it is a fully supervised method that has no Unseen classes during test time; 2) it also uses MRI and histopathology features from available data while we generate synthetic features to overcome unavailability of one data modality.

2 Method

2.1 Feature Extraction And Transformation:

Figure 1 depicts our overall proposed workflow, which has 3 networks for: feature extraction, feature transformation and self supervised feature synthesis. Let the training set consist of histopathology and MR images from PCa cases with known Gleason grades. We train a network that can correctly predict seen and unseen Gleason grades using MR images only. Let the dataset of ‘Seen’ and ‘Unseen’ classes be \( S, U \) and their corresponding labels be \( Y_s, Y_u \). \( Y = Y_s \cup Y_u \), and \( Y_s \cap Y_u = \emptyset \). Previous works [16] show that generating feature vectors, instead of images, performs better for GZSL classification since output images of generative models can be blurry, especially with multiple objects (e.g., multiple cells.
Fig. 1: **Training Workflow:** Feature extraction from MR and digital pathology images generates respective feature vectors \( F_{MRI} \) and \( F_{DP} \). \( F_{MRI} \) is input to a feature synthesis network to generate new MR features for ‘Seen’ and ‘Unseen’ classes, which are passed through the feature transformation network to obtain corresponding \( F_{DP} \). Combined MR and histopathology features are used to train a softmax classifier for identifying ‘Seen’ and ‘Unseen’ test classes. A self-supervised module contributes to the sample generation step through \( \mathcal{L}_{CPC} \).

in histopathology images. Additionally, generating high-resolution histopathology images from low resolution and noisy MRI is challenging, while finding a transformation between their feature vectors is much more feasible.

We train two separate ResNet-50 networks [22] as feature extractors for MR and DP images. Histopathology image feature extractor \( FE_{DP} \) is pre-trained on the PANDA dataset [14] that has a large number of whole slide images for PCa classification. \( FE_{MRI} \) is pre-trained with the PROMISE12 challenge dataset [40] in a self-supervised manner. Since PROMISE12 is for prostate segmentation from MRI and does not have classification labels, we use a pre-text task of predicting if an image slice has the prostate or not. Gleason grades of MRI are the same as corresponding histopathology images. The images are processed through the convolution blocks and the 1000 dimensional output of the last FC layer is the feature vector for MRI \( (F_{MRI}) \) and pathology images \( (F_{DP}) \).

**Feature Transformation** is achieved using CycleGANs [65, 93, 94, 96, 163] to learn mapping functions \( G : X \rightarrow Y \) and \( F : Y \rightarrow X \), between feature vectors \( X = F_{MRI} \) and \( Y = F_{DP} \). Adversarial discriminator \( D_X \) differentiates between real features \( F_{DP} \) and generated features \( \hat{F}_{DP} \), and \( D_Y \) distinguishes between \( F_{MRI} \) and \( \hat{F}_{MRI} \). The adversarial loss (Eqn. 1) and cycle consistency loss (Eqn. 2) are,

\[
\begin{align*}
L_{adv}(G, D_Y) &= \mathbb{E}_y [\log D_Y(y)] + \mathbb{E}_x [\log(1 - D_Y(G(x)))] , \\
L_{adv}(F, D_X) &= \mathbb{E}_x [\log D_X(x)] + \mathbb{E}_y [\log(1 - D_X(F(y)))] .
\end{align*}
\]
\[ L_{\text{cycle}}(G, F) = E_z \| F(G(x)) - x \|_1 + E_y \| G(F(y)) - y \|_1. \]  

**Network Training**: is done using \( L_{\text{adv}}(G, D_Y) + L_{\text{adv}}(F, D_X) + L_{\text{cycle}}(G, F) \). Generator \( G \) is a multi-layer perceptron (MLP) with a hidden layer of 4096 nodes having LeakyReLU \[138]. The output layer with 2048 nodes has ReLU activation \[138]. \( G \)'s weights are initialized with a truncated normal of \( \mu = 0, \sigma = 0.01 \), and biases initialized to 0. Discriminator \( D \) is an MLP with a hidden layer of 2048 nodes activated by LeakyReLU, and the output layer has no activation. \( D \)'s initialization is the same as \( G \), and we use Adam optimizer \[31].

### 2.2 CVAE Based Feature Generator Using Self Supervision

The conditional variational autoencoder (CVAE) generator synthesizes feature vectors \( F_{\text{output}}^{\text{output}} \) of desired class \( c_{\text{MRI}}^{\text{output}} \), given input features \( F_{\text{MRI}}^{\text{input}} \), with known class \( c_{\text{MRI}}^{\text{input}} \). Let \( x = F_{\text{MRI}}^{\text{input}} \), \( z = F_{\text{MRI}}^{\text{output}} \), and \( c = c_{\text{MRI}}^{\text{output}} \). The CVAE loss is,

\[
\min_{\theta_{E}, \theta_{P}} \mathcal{L}_{CVAE} + \lambda_{c} \cdot \mathcal{L}_{c} + \lambda_{\text{reg}} \cdot \mathcal{L}_{\text{reg}} + \lambda_{E} \cdot \mathcal{L}_{E} + \lambda_{\text{CPC}} \cdot \mathcal{L}_{\text{CPC}}
\]  

(3)

Denoting CVAE encoder as \( p_{E}(z|x) \) with parameters \( \theta_{E} \), and the regressor output distribution as \( p_{R}(c|x) \), the CVAE loss is,

\[
\mathcal{L}_{CVAE}(\theta_{E}, \theta_{G}) = -\mathbb{E}_{p_{E}(z|x), p(c|x)} \left[ \log p_{G}(x|z, c) \right] + KL(p_{E}(z|x)||p(z))
\]  

(4)

\( \mathbb{E}_{p_{E}(z|x), p(c|x)} \) is the generator’s reconstruction error, and KL divergence, \( KL(,\) ), encourages CVAE posterior (the encoder) to be close to the prior. Encoder \( p_{E}(z|x) \), conditional decoder/generator \( p_{G}(x|z, c) \), and regressor \( p_{R}(c|x) \) are modeled as Gaussian distributions. The latent code \((z, c)\) is represented by disentangled representations \( p_{E}(z|x) \) and \( p_{R}(c|x) \) to avoid posterior collapse \[24\].

**Regression/Discriminator Module - REG\text{Synth}**: is a feedforward neural network mapping input feature vector \( x \in \mathbb{R}^{D} \) to its corresponding class-value \( c \in \mathbb{R}^{1} \). \( REG\text{Synth} \) is a probabilistic model \( p_{R}(c|x) \) with parameters \( \theta_{R} \) and is trained using supervised (\( \mathcal{L}_{\text{sup}} \)) and unsupervised (\( \mathcal{L}_{\text{unsup}} \)) losses:

\[
\min_{\theta_{R}} \mathcal{L}_{R} = \mathcal{L}_{\text{sup}} + \lambda_{R} \cdot \mathcal{L}_{\text{unsup}}
\]  

(5)

\( \lambda_{R} = 0.2 \) and \( \mathcal{L}_{\text{sup}}(\theta_{R}) = -\mathbb{E}_{(x_n, c_n)} \left[ p_{R}(c_n|x_n) \right] \) is defined on labeled examples \((x_n, c_n)_{n=1}^{N}\) from the seen class. \( \mathcal{L}_{\text{unsup}}(\theta_{R}) = -\mathbb{E}_{p_{D}(\tilde{z}|z, c)p(z)p(c)} \left[ p_{R}(c|\tilde{z}) \right] \) is defined on synthesized examples \( \tilde{z} \) from the generator. \( \mathcal{L}_{\text{unsup}} \) is obtained by sampling \( z \) from \( p(z) \), and class-value \( c \) sampled from \( p(c) \) to generate an exemplar \( p_{\theta_{R}}(\tilde{z}|z, c) \), and we calculate the expectation w.r.t. these distributions.

**Discriminator-Driven Learning**: The error back-propagated from \( REG\text{Synth} \) improves quality of synthetic samples \( \tilde{x} \) making them similar to the desired output class-value \( c \). This is achieved using multiple loss functions. The first generates samples whose regressed class value is close to the desired value,

\[
\mathcal{L}_{c}(\theta_{G}) = -\mathbb{E}_{p_{G}(\tilde{z}|z, c)p(z)p(c)} \left[ \log p_{R}(c|\tilde{z}) \right]
\]  

(6)
The second term draws samples from prior \( p(z) \) and combines with class-value from \( p(c) \), to ensure the synthesized features are similar to the training data,

\[
\mathcal{L}_{Reg}(\theta_G) = -\mathbb{E}_{p(z)p(c)} \left[ \log p_G(\hat{x}|z, c) \right]
\]  

(7)

The third loss term ensures independence (disentanglement) \[24\] of \( z \) from the class-value \( c \). The encoder ensures that the sampling distribution and the one obtained from the generated sample follow the same distribution.

\[
\mathcal{L}_E(\theta_G) = -\mathbb{E}_{\hat{x} \sim p_G(\hat{x}|z, c)} KL \left[ \log p_E(z|\hat{x}) || q(z) \right]
\]  

(8)

The distribution \( q(z) \) could be the prior \( p(z) \) or the posterior from a labeled sample \( p(z|x_n) \).

**Self Supervised Loss:** Gleason grades have a certain ordering, i.e., grade 3 indicates higher severity than grade 1, and grade 5 is higher than grade 3. Contrastive Predictive Coding (CPC) \[140\] learns self-supervised representations by predicting future observations from past ones and requires that observations be ordered in some dimension. Inspired by CPC we train our network to predict features of desired Gleason grade from input features of a different grade. From the training data we construct pairs of \( \{F_{input \ MRI}, c_{input \ MRI}, F_{output \ MRI}, c_{output \ MRI}\} \), the input and output features and desired class label value \( c_{output \ MRI} \) of synthesized vector.

Since the semantic gap between \( F_{input \ MRI} \) and \( F_{output \ MRI} \) may be too large, we use random transformations to first generate intermediate representation of positive \( z^+ \), anchor \( z^a \) and negative \( z^- \) features using the mutual information-based AMDIM approach of \[2\]. AMDIM ensures that the mutual information between similar samples \( z^+, z^a \) is high while for dissimilar samples \( z^-, z^a \) it is low, where \( z = F_{output \ MRI} \). The CPC objective (Eqn. 9) evaluates the quality of the predictions using a contrastive loss where the goal is to correctly recognize the synthetic vector \( z \) among a set of randomly sampled feature vectors \( z_I = \{ z^+, z^a, z^- \} \).

\[
\mathcal{L}_{CPC} = -\sum \log \frac{\exp(F_{input \ MRI}^T F_{output \ MRI})}{\sum \exp(F_{input \ MRI}^T F_{output \ MRI}) + \sum \exp(F_{input \ MRI}^T F_{output \ MRI})}
\]  

(9)

This loss is the InfoNCE inspired from Noise-Contrastive Estimation \[21, 137\] and maximizes the mutual information between \( c \) and \( z \) \[140\]. By specifying the desired class label value of synthesized vector and using it to guide feature generation in the CVAE framework we avoid the pitfalls of unconstrained and unrealistic feature generation common in generative model based GZSL (e.g., \[41, 161\]).

**Training And Implementation:** Our framework was implemented in PyTorch. The CVAE Encoder has two hidden layers of 2000 and 1000 units respectively while the CVAE Generator is implemented with one hidden layer of 1000 hidden units. The Regressor has only one hidden layer of 800 units. We choose Adam \[31\] as our optimizer, and the momentum is set to \((0.9, 0.999)\). The learning rate for CVAE and Regressor is 0.0001. First the CVAE loss (Eqn. 4) is
pre-trained followed by joint training of regressor and encoder-generator pair in optimizing Eqn. 7 and Eqn. 3 till convergence. Hyperparameter values were chosen using a train-validation split with $\lambda_R = 0.1, \lambda_c = 0.1, \lambda_{reg} = 0.1, \lambda_E = 0.1,$ and $\lambda_{CPC} = 0.2$. Training the feature extractor for 50 epochs takes 12 hours and the feature synthesis network for 50 epochs takes 17 hours, all on a single NVIDIA V100 GPU (32 GB RAM).

**Evaluation Protocol:** The seen class $S$ has samples from 2 or more Gleason grades, and the unseen class $U$ contains samples from remaining classes. 80 - 20 split of $S$ is done into $S_{Train}/S_{Test}$. $F_{MRI}$ is synthesized from $S + U$ using the CVAE and combined with the corresponding synthetic $F_{DP}$ to obtain a single feature vector for training a softmax classifier minimizing the negative log-likelihood loss. Following standard practice for GZSL, average class accuracies are calculated for two settings: 1) Setting A: training is performed on synthesized samples of $S + U$ classes and test on $S_{Test}$. 2) Setting B: training is performed on synthesized samples of $S + U$ classes and test on $U$. Following GZSL protocol we report the harmonic mean: $H = \frac{2 \times Acc_U \times Acc_S}{Acc_U + Acc_S}$; $Acc_S$ and $Acc_U$ are classification accuracy of images from seen (setting A) and unseen (setting B) classes respectively.

## 3 Experimental Results

**Dataset Details:** We use images from 321 patients (48 - 70 years; mean: 58.5 years) undergone prostate surgery with pre-operative T2-w and Apparent Diffusion Coefficient MRI, and post-operative digitized histopathology images. To ensure prostate tissue is sectioned in same plane as T2w MRI custom 3D printed molds were used. Majority votes among three pathologists provided Gleason grades was the consensus annotation. Pre-operative MRI and histopathology images were registered [145] to enable accurate mapping of cancer labels. We have the following classes: Class 1: Grade 3, 67 patients, Class 2: Grades 3 + 4/4 + 3, 60 patients, Class 3: Grade 4, 74 patients, Class 4: Grades 4 + 5/5 + 4, 57 patients, Class 5: Grade 5, 63 patients. In the supplementary we show results for the Kaggle DR challenge [17] and PANDA challenge [14].

**Pre-processing:** Histopathology images were smoothed with a Gaussian filter ($\sigma = 0.25$). They were downsized to $224 \times 224$ with X-Y resolution $0.25 \times 0.25 \text{mm}^2$. The T2w images, prostate masks, and Gleason labels are projected on the corresponding downsized histopathology images and resampled to the same X-Y resolution. This ensures corresponding pixels in each modality represents the same physical area. MR images were normalized using histogram alignment [139]. The training, validation, and test sets had 193/64/64 patients.

We compare results of our method MM$_{GZSL}$ (Multimodal GZSL) with different feature generation based GZSL methods: 1) CVAE based feature synthesis method of [25]; 2) GZSL using over complete distributions [30]; 3) self-supervised learning GZSL method of [160]; 4) cycle-GAN GZSL method of [16]; 5) FSL-
fully supervised learning method of [6] using the same data split, actual labels of ‘Unseen’ class and almost equal representation of all classes.

Table 1: GZSL and Ablation Results: Average classification accuracy (%) and harmonic mean accuracy of generalized zero-shot learning when test samples are from Seen (Setting \(A\)) or unseen (Setting \(B\)) classes. Mean and variance are reported when the number of classes in the ‘Seen’ set is 3. \(p\) values are with respect to Harmonic Mean of MM\(_{GZSL}\).

| Comparison Methods | Acc\(_S\) | Acc\(_U\) | H | p | Sen\(_S\) | Spe\(_S\) | Sen\(_U\) | Spe\(_U\) |
|--------------------|-----------|-----------|---|---|-----------|-----------|-----------|-----------|
| MM\(_{GZSL}\)     | 83.6(2.4) | 81.7(3.0) | 82.6(2.8) | - | 84.1(3.1) | 82.9(2.6) | 81.2(3.0) | 80.1(3.3) |
| 25                 | 80.3(3.5) | 73.4(3.6) | 76.7(2.8) | 0.002 | 81.2(2.6) | 79.9(3.5) | 74.1(3.2) | 72.8(3.4) |
| 30                 | 80.6(3.4) | 72.8(3.0) | 76.5(3.2) | 0.001 | 81.1(2.9) | 80.0(3.2) | 73.5(3.1) | 72.1(3.4) |
| 160                | 81.1(2.9) | 73.2(3.2) | 76.9(3.1) | 0.001 | 81.8(3.5) | 80.7(3.1) | 74.0(3.5) | 72.9(3.7) |
| 16                 | 81.2(3.7) | 72.8(3.8) | 76.7(3.8) | 0.004 | 81.8(3.1) | 80.7(3.4) | 73.1(4.0) | 71.9(4.2) |
| FSL               | 83.9(2.2) | 83.3(2.5) | 83.5(2.3) | 0.01 | 84.9(2.4) | 83.5(2.6) | 83.7(2.8) | 82.5(2.6) |

### 3.1 Generalized Zero Shot Learning Results

Table 1 summarizes the results of our algorithm and other methods when the Seen set has samples from 3 classes. The numbers are an average of 5 runs. Samples from 3 labeled classes presents the optimum scenario balancing high classification accuracy, and generation of representative synthetic samples. Setting \(A\) does better than setting \(B\). Since GZSL is a very challenging problem, it is expected that classification performance on Unseen classes will not match those of Seen classes. MM\(_{GZSL}\)’s performance is closest to FSL. Since FSL has been trained with all classes in training and test sets it gives the best results.

We use the McNemar test and determine that the difference in Acc\(_S\) of MM\(_{GZSL}\) and FSL is not significant \((p = 0.062)\) although the corresponding values for Acc\(_U\) are significant \((p = 0.031)\) which is not surprising since real Unseen examples have not been encountered in GZSL. Since MM\(_{GZSL}\)’s performance is closest to FSL for Unseen classes, it demonstrates MM\(_{GZSL}\)’s effectiveness in generating realistic features of unseen classes. We refer the reader to the supplementary material for additional results (e.g. using different number of classes in the Seen dataset). The individual Per Class mean accuracy and
Ablation Studies: Table 1 shows ablation results where each row denotes a specific setting without the particular term in the final objective function in Eqn 3 - e.g., MM_{wCPC} denotes our proposed method MM_{GZSL} without the self-supervised loss \( \mathcal{L}_{CPC} \). MM_{wCPC} shows the worst performance indicating \( \mathcal{L}_{CPC} \)’s correspondingly higher contribution than other terms. The \( p \)–values indicate each term’s contribution is significant for the overall performance of MM_{GZSL} and excluding any one leads to significant performance degradation.

We also show in Table 1 the result of using: 1) only the synthetic MR features (MM_{MR}); 2) only digital histopathology features (MM_{DP}) obtained by transforming \( F_{MRI} \) to get \( F_{DP} \). MM_{DP} gives performance metrics closer to MM_{GZSL}, which indicates that the digital histopathology images provide highly discriminative information compared to MR images. However, MR images also have a notable contribution, as indicated by the \( p \)-values. In another set of experiments we redesign the GZSL experiments to generate synthetic histopathology features \( F_{DP} \) instead of \( F_{MRI} \) and then transforming them to get MR features. We obtain very similar performance (Acc_S = 83.7, Acc_U = 80.8, H = 82.2) to the original MM_{GZSL} setting. This demonstrates that cycle GAN based feature transformation network does a good job of learning accurate histopathology features from the corresponding MR features.

Visualization of Synthetic Features: Figure 2 (a) shows t-SNE plot of real data features where the classes are spread over a wide area, with overlap amongst consecutive classes. Figures 2 (b,c,d) show, respectively, distribution of synthetic features generated by MM_{GZSL}, MM_{wCPC} and \([160]\). MM_{GZSL} features are the most similar to the original data. MM_{wCPC} and \([160]\) synthesize sub-optimal feature representation of actual features, resulting in poor classification performance on unseen classes.

4 Conclusion

We propose a GZSL approach without relying on class attribute vectors. Our novel method can accurately predict Gleason grades from MR images with lower resolution and less information content than histopathology images. This has the potential to improve accuracy of early detection and staging of PCa. A self-supervised component ensures the semantic gap between Seen and Unseen classes is easily covered. The distribution of synthetic features generated by our method are close to the actual distribution, while removing the self-supervised term results in unrealistic distributions. Results show our method’s superior performance and synergy between different loss terms leads to improved GZSL
classification. We observe failure cases where the acquired MR images are not of sufficiently good resolution to allow accurate registration of histopathology and MRI. Future work will aim to address this issue.

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