

## Appendix A. Discussion

We can extend the definition of robustness to triplet-based metric learning algorithms, i.e., we take the admissible triplet set  $\text{trip}_{\mathbf{s}}$  of  $s$  such that  $(s_1, s_2, s_3) \in \text{trip}_{\mathbf{s}}$ . The robustness property means  $s_1$  and  $s_2$  share the same label while  $s_1$  and  $s_3$  have different ones, with the interpretation that  $s_1$  must be more similar to  $s_2$  than to  $s_3$ , formulated as follows:  $\forall (s_1, s_2, s_3) \in \text{trip}_{\mathbf{s}}, \forall z_1, z_2, z_3 \in \mathcal{Z}, \forall i, j, k \in [k]$ , if  $s_1, z_1 \in C_i, s_2, z_2 \in C_j$  and  $s_3, z_3 \in C_k$  then

$$|\ell(\mathcal{A}_{\text{trip}_{\mathbf{s}}}, s_1, s_2, s_3) - \ell(\mathcal{A}_{\text{trip}_{\mathbf{s}}}, z_1, z_2, z_3)| \leq \epsilon(\text{trip}_{\mathbf{s}}). \quad (\text{A.1})$$

Following this definition, Proposition 3 can be easily extended to obtain the following generalization bound

$$|\mathcal{L}(\mathcal{A}_{\text{trip}_{\mathbf{s}}}) - \mathcal{L}_{\text{emp}}(\mathcal{A}_{\text{trip}_{\mathbf{s}}})| \leq \epsilon(\text{trip}_{\mathbf{s}}) + 3B \sqrt{\frac{2K \ln 2 + 2 \ln 1/\delta}{n}}. \quad (\text{A.2})$$

For triplet based metric learning algorithms, by following the definition of robustness given by Eq. (A.1) and adapting straightforwardly the losses to triplets such that they output zero for non-admissible ones, we can obtain the following bound

$$|\mathcal{L}(\mathcal{A}_{\mathbf{s}}) - \mathcal{L}_{\text{emp}}(\mathcal{A}_{\mathbf{s}})| \leq \epsilon(\mathbf{s}) + \xi(\mathcal{A}_{\mathbf{s}}) \left( (3\sqrt{2} + 3) \sqrt{\frac{|\mathcal{T}_{\mathbf{s}}| \ln(2K/\delta)}{n}} + \frac{2|\mathcal{T}_{\mathbf{s}}| \ln(2K/\delta)}{n} \right). \quad (\text{A.3})$$

Using triplet-based robustness, consider algorithms of the following form

$$\min_{\mathbf{M} \geq 0} c \|\mathbf{M}\| + \frac{1}{|\text{trip}_{\mathbf{s}}|} \sum_{(s_i, s_j, s_k) \in \text{trip}_{\mathbf{s}}} [1 - (x_i - x_k)^T \mathbf{M} (x_i - x_k) + (x_i - x_j)^T \mathbf{M} (x_i - x_j)]_+,$$

where  $\|\mathbf{M}\| = \|\mathbf{M}\|_{\mathcal{F}}$  in Example 4 or  $\|\mathbf{M}\| = \|\mathbf{M}\|_{1,2}$  in Example 5. These methods are  $(\mathcal{N}(\gamma, \mathbb{Z}, \|\cdot\|_2), 16UR_y g_0/c)$ -robust.

## Appendix B. Additional Proofs

In this section, we present the proof of Lemma 17, Lemma 18 and Lemma 19. Recall that  $C_i$  is defined in Definition 1.

**Proof** [Proof of Lemma 17] By the definition of  $\mathcal{L}$  and  $\mathcal{L}_{\text{emp}}$ , we know

$$\begin{aligned}
& |\mathcal{L}(\mathcal{A}_{\mathbf{s}}) - \mathcal{L}_{\text{emp}}(\mathcal{A}_{\mathbf{s}})| \\
&= \left| \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z')] - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_{\mathbf{s}}, z_i, z_j) \right| \\
&= \left| \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] p_i p_j - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_{\mathbf{s}}, z_i, z_j) \right| \\
&\stackrel{(a)}{\leq} \left| \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] p_i p_j - \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] p_i \frac{|\mathcal{I}_j|}{n} \right| \\
&+ \left| \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] p_i \frac{|\mathcal{I}_j|}{n} - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_{\mathbf{s}}, z_i, z_j) \right| \\
&\stackrel{(b)}{\leq} \left| \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] p_i (p_j - \frac{|\mathcal{I}_j|}{n}) \right| \\
&+ \left| \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] p_i \frac{|\mathcal{I}_j|}{n} - \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i| |\mathcal{I}_j|}{n^2} \right| \\
&+ \left| \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i| |\mathcal{I}_j|}{n^2} - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_{\mathbf{s}}, z_i, z_j) \right|,
\end{aligned}$$

where inequalities (a) and (b) are due to the triangle inequality. By the following symmetrical property of metric  $\mathcal{A}_{\mathbf{s}}$ , we know

$$\begin{aligned}
& \left| \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_j|}{n} (p_i - \frac{|\mathcal{I}_i|}{n}) \right| \\
&= \left| \sum_{i,j \in [K]} \mathbb{E}_{z, z' \sim \mu}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i|}{n} (p_j - \frac{|\mathcal{I}_j|}{n}) \right|.
\end{aligned}$$

It then follows that

$$\begin{aligned}
 & |\mathcal{L}(\mathcal{A}_s) - \mathcal{L}_{\text{emp}}(\mathcal{A}_s)| \\
 & \leq \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] p_i (p_j - \frac{|\mathcal{I}_j|}{n}) \right| \\
 & + \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_j|}{n} (p_i - \frac{|\mathcal{I}_i|}{n}) \right| \\
 & + \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i| |\mathcal{I}_j|}{n^2} - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_s, z_i, z_j) \right| \\
 & \leq \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] p_j (p_i - \frac{|\mathcal{I}_i|}{n}) \right| \\
 & + \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_j|}{n} (p_i - \frac{|\mathcal{I}_i|}{n}) \right| \\
 & + \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i| |\mathcal{I}_j|}{n^2} - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_s, z_i, z_j) \right| \\
 & \leq \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] (p_j + \frac{|\mathcal{I}_j|}{n}) \left| p_i - \frac{|\mathcal{I}_i|}{n} \right| \\
 & + \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i| |\mathcal{I}_j|}{n^2} - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_s, z_i, z_j) \right|.
 \end{aligned}$$

The proof is completed. ■

**Proof** [Proof of Lemma 18] By definition, we have  $\sum_{i=1}^K |\mathcal{I}_i| = n$  and  $\sum_{i=1}^K p_i = 1$ . Then,

$$\begin{aligned}
 & \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i| |\mathcal{I}_j|}{n^2} - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_s, z_i, z_j) \right| \\
 & \leq \frac{1}{n^2} \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] |\mathcal{I}_i| |\mathcal{I}_j| - \sum_{i,j=1}^n \ell(\mathcal{A}_s, z_i, z_j) \right| \\
 & = \frac{1}{n^2} \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} \sum_{z_p \in C_i, z_q \in C_j} [\ell(\mathcal{A}_s, z, z') | z \in C_i, z' \in C_j] - \sum_{i,j \in [K]} \sum_{z_p \in C_i, z_q \in C_j} \ell(\mathcal{A}_s, z_p, z_q) \right| \\
 & \leq \frac{1}{n^2} \sum_{i,j \in [K]} \sum_{z_p \in C_i, z_q \in C_j} \max_{z \in C_i, z' \in C_j} |\ell(\mathcal{A}_s, z, z') - \ell(\mathcal{A}_s, z_p, z_q)| \\
 & \leq \max_{i,j \in [n]} \max_{z_p, z \in C_i, z_q, z' \in C_j} |\ell(\mathcal{A}_s, z, z') - \ell(\mathcal{A}_s, z_p, z_q)|.
 \end{aligned}$$
■

**Proof** [Proof of Lemma 19] First, define  $\hat{\mathcal{I}}_k := \{i \in [n] : z_i \in \hat{\mathbf{s}}, z_i \in C_k\}$ ,  $\hat{\mathbf{s}}$  is defined in definition 12. Then starting from the second to the last step of Lemma 18, we know

$$\begin{aligned}
& \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i| |\mathcal{I}_j|}{n^2} - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_{\mathbf{s}}, z_i, z_j) \right| \\
& \leq \frac{1}{n^2} \sum_{i,j \in [K]} \sum_{z_p \in C_i, z_q \in C_j} \max_{z \in C_i, z' \in C_j} |\ell(\mathcal{A}_{\mathbf{s}}, z, z') - \ell(\mathcal{A}_{\mathbf{s}}, z_p, z_q)| \\
& \leq \frac{1}{n^2} \sum_{i,j \in [K]} \sum_{p \in \hat{\mathcal{I}}_i, q \in \hat{\mathcal{I}}_j} \max_{z \in C_i, z' \in C_j} |\ell(\mathcal{A}_{\mathbf{s}}, z, z') - \ell(\mathcal{A}_{\mathbf{s}}, z_p, z_q)| \\
& + \frac{1}{n^2} \sum_{i,j \in [K]} \sum_{\neg(p \in \hat{\mathcal{I}}_i, q \in \hat{\mathcal{I}}_j)} \max_{z \in C_i, z' \in C_j} |\ell(\mathcal{A}_{\mathbf{s}}, z, z') - \ell(\mathcal{A}_{\mathbf{s}}, z_p, z_q)| \\
& \leq \frac{1}{n^2} \sum_{i,j \in [K]} \sum_{p \in \hat{\mathcal{I}}_i, q \in \hat{\mathcal{I}}_j} \max_{z \in C_i, z' \in C_j} |\ell(\mathcal{A}_{\mathbf{s}}, z, z') - \ell(\mathcal{A}_{\mathbf{s}}, z_p, z_q)| \\
& + \frac{1}{n^2} \sum_{i,j \in [K]} \sum_{\neg(p \in \hat{\mathcal{I}}_i, q \in \hat{\mathcal{I}}_j)} \max_{z \in C_i, z' \in C_j} |\ell(\mathcal{A}_{\mathbf{s}}, z, z') - \ell(\mathcal{A}_{\mathbf{s}}, z_p, z_q)|.
\end{aligned}$$

Recall that  $\ell$  is positive, and the weak robustness properties. It then follows that

$$\begin{aligned}
& \left| \sum_{i,j \in [K]} \mathbb{E}_{z,z' \sim \mu} [\ell(\mathcal{A}_{\mathbf{s}}, z, z') | z \in C_i, z' \in C_j] \frac{|\mathcal{I}_i| |\mathcal{I}_j|}{n^2} - \frac{1}{n^2} \sum_{i,j=1}^n \ell(\mathcal{A}_{\mathbf{s}}, z_i, z_j) \right| \\
& \leq \frac{|\hat{\mathbf{s}}^2|}{n^2} + \frac{n^2 - |\hat{\mathbf{s}}^2|}{n^2} \xi(\mathcal{A}_{\mathbf{s}}).
\end{aligned}$$

The proof is completed. ■

## Appendix C. Notation Index

$\mathcal{Z}$  Sample space, defined as  $\mathcal{X} \times \mathcal{Y}$ .

$\mathcal{X}$  Input space, a subset of  $\mathbb{R}^d$ , where  $d$  is the dimensionality of the input space.

$\mathcal{Y}$  Output space, a subset of  $\mathbb{R}$ .

$\mu$  Unknown probability distribution over  $\mathcal{Z}$ .

$\mathbf{s}$  Training dataset,  $\mathbf{s} = (z_1, \dots, z_n)$ .

$n$  Number of training examples.

$z_i$  Individual training example,  $z_i \in \mathcal{Z}$ .

$\mathcal{F}$  Model space.

$f$  Model in model space  $\mathcal{F}$ ;  $f : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$  in pairwise learning or  $f : \mathcal{X} \mapsto \mathbb{R}$  in pointwise learning.

$\ell$  Loss function;  $\ell : \mathcal{F} \times \mathcal{Z} \times \mathcal{Z} \mapsto \mathbb{R}^+$ .

$\ell(f, z, z')$  Loss of model  $f$  on example pair  $(z, z')$  with  $\ell(f, z, z) = 0$ .

$\mathcal{L}(f)$  Population risk:  $\mathbb{E}_{z, z' \sim \mu}[\ell(f, z, z')]$ .

$\mathcal{L}_{\text{emp}}(f)$  Empirical risk;  $\frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \ell(f, z_i, z_j)$ .

$\mathcal{A}$  Optimization algorithm.

$\mathcal{A}_{\mathbf{s}}$  Model learned by applying  $\mathcal{A}$  to dataset  $\mathbf{s}$ .

$B$  Upper bound on loss:  $\ell(f, z) \leq B$  for all  $f \in \mathcal{F}, z \in \mathcal{Z}$ .

$|\mathcal{B}|$  Cardinality (number of elements) of the set  $\mathcal{B}$

$[n]$  Set of integers  $\{1, \dots, n\}$  where  $n \in \mathbb{N}$

$\epsilon(\cdot)$  Robustness parameter function  $\epsilon : \mathcal{Z}^n \mapsto \mathbb{R}_+$

$K$  Number of partitions of Sample space  $\mathcal{Z}$ .

$\{C_k\}_{k=1}^K$  Partition of  $\mathcal{Z}$  into  $K$  disjoint sets

$\mathcal{T}_{\mathbf{s}}$  Set of partition indices with at least one training example:  $\{k \in [K] : |\mathcal{I}_k^{\mathbf{s}}| \geq 1\}$

$\mathcal{T}_{\mathbf{s}}^c$  Complement of  $\mathcal{T}_{\mathbf{s}}$ :  $\{k \in [K] : |\mathcal{I}_k^{\mathbf{s}}| = 0\}$  (partitions with no training examples)

$\mathcal{I}_k^{\mathbf{s}}$  Index set of examples in  $\mathbf{s}$  belonging to  $C_k$ :  $\{i \in [n] : z_i \in C_k\}$

$p_k$  Probability  $\mathbb{P}(z \in C_k)$

$p$  Probability vector  $(p_1, \dots, p_K)$

$\xi(\mathcal{A}_{\mathbf{s}})$  Conditional expected loss:  $\max_{i, j \in [K]} \mathbb{E}_{z, z'}[\ell(\mathcal{A}_{\mathbf{s}}, z, z') \mid z \in C_i, z' \in C_j]$

$\delta$  Confidence parameter ( $\delta \in (0, 1)$ )

$\alpha_k(f)$  Maximum conditional expected loss for class  $k$ :  $\max_{j \in [n]} \mathbb{E}_{z, z'}[\ell(f, z, z') \mid z \in C_k, z' \in C_j]$

$\alpha_{\mathcal{T}_{\mathbf{s}}}(f)$  Maximum  $\alpha_k$  over active partitions:  $\max_{k \in \mathcal{T}_{\mathbf{s}}} \alpha_k(f)$

$\alpha_{\mathcal{T}_{\mathbf{s}}^c}(f)$  Maximum  $\alpha_k$  over inactive partitions:  $\max_{k \in \mathcal{T}_{\mathbf{s}}^c} \alpha_k(f)$

$\mathcal{Q}_1 = \sum_{k \in \mathcal{T}_{\mathbf{s}}} (\alpha_{\mathcal{T}_{\mathbf{s}}^c}(\mathcal{A}_{\mathbf{s}}) + \sqrt{2} \alpha_k(\mathcal{A}_{\mathbf{s}}) \sqrt{\frac{|\mathcal{I}_k^{\mathbf{s}}|}{n}})$

$\mathcal{Q}_2 = \alpha_{\mathcal{T}_{\mathbf{s}}^c}(\mathcal{A}_{\mathbf{s}}) |\mathcal{T}_{\mathbf{s}}| + \sum_{k \in \mathcal{T}_{\mathbf{s}}} \alpha_k(\mathcal{A}_{\mathbf{s}})$

$\hat{p}_n(\cdot)$  Pseudo-robustness function:  $\hat{p}_n : (\mathcal{Z} \times \mathcal{Z})^n \rightarrow \{1, \dots, n^2\}$

$\mathbf{s}^2$  Full set of training pairs:  $\{(z_i, z_j) : z_i, z_j \in \mathbf{s}\}$  (size  $n^2$ )

$\hat{\mathbf{s}}^2$  Subset of pairwise training dataset  $\mathbf{s}^2$ .

$\epsilon(\mathbf{s}^2)$  Robustness parameter as function of training pairs