

COOD: Combined out-of-distribution detection using multiple measures for anomaly & novel class detection in large-scale hierarchical classification

Supplementary Material

8. Appendix

8.1. Taxon distance

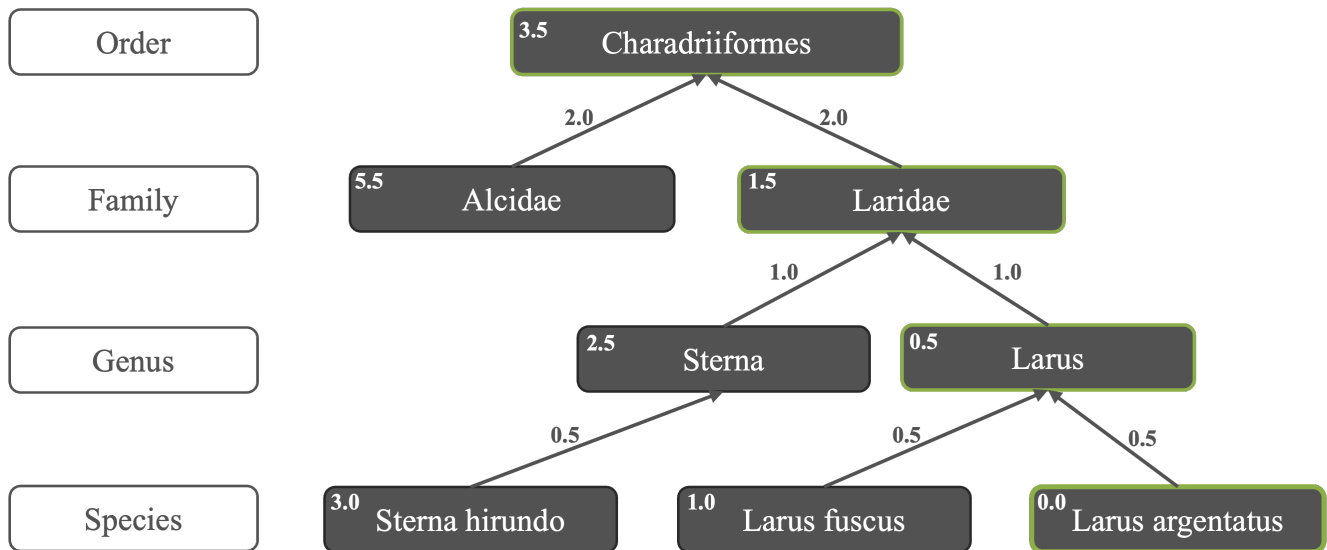


Figure 5. Taxon distance. Shows a part of a hierarchical class tree where taxa (biological classes) make up the nodes. The taxon distance (TD) is defined as the sum of the number of weighted edges between two nodes in the tree (the first node in the example is *Larus argentatus*). The weights are used to ensure that distances higher in the tree are larger, matching with the concept of broader groups. Per definition the distance between to species in the same genus = 1.0, e.g. $TD(\text{Larus argentatus}, \text{Larus fuscus}) = 1$

8.2. Mathematical definitions

Name	Definition	Symbol
Data point	x_i from dataset \mathcal{D}	x
Feature	$f(x)$, (image) feature for x	f
Logits	$g = W * f + b$, where W is the classification weight matrix, b the classification bias, and g_c is the linear output for the c^{th} class	g_c
Temperature scaled linear class probability	$p_T(x, T) = \frac{e^{g_c(x)/T}}{\sum_{c=1}^{ \mathcal{C} } e^{g_c(x)/T}}$, also known as <i>SoftMax</i> , where \mathcal{C} indicates set of classes and T is the temperature scale factor	p_T
Linear class probability	$p_c(x) = p_T(x, 1.0)$	p
Feature distance	$d(f_i, f_j)$, without loss of generality we assume low d means more similar features	d
n-th nearest neighbor	$\mathcal{N}_n(x)$, as found by kNN search, per definition $\mathcal{N}_1 = \operatorname{argmin}_{x_j \in X} d(x, x_j)$, assuming $x \notin X$	\mathcal{N}_n
True class	$\mathcal{T}(x)$, gives true class for x	$\mathcal{T}(x)$
kNN class histogram	$h_{c, \mathcal{N}}(x) = \sum_{n=1}^k \mathbf{1}[\mathcal{T}(\mathcal{N}_n) = c]$, for all $c \in \mathcal{C}$ where $\mathbf{1}[\cdot]$ is the indicator function	$h_{\mathcal{N}}$
kNN class probability vector	$\frac{1}{k} h_{\mathcal{N}}$	$p_{\mathcal{N}}$
Entropy	$H(p) = -\sum_{i=1}^n p_i \log_2(p_i)$, where p is an arbitrary probability vector	H

Table 6. Basic mathematical definitions

OOD Measure	Definition	Symbol
Avg. distance among NN	$\frac{1}{k(k-1)} \sum_n^k \sum_{n \neq m}^k d(f(\mathcal{N}_m), f(\mathcal{N}_n))$	\bar{D}
Avg. distance to NN	$\frac{1}{k} \sum_n^k d(f, f(\mathcal{N}_n))$	\bar{d}
Distance to 1st NN	$d(f, f(\mathcal{N}_1))$	d_1
Distance to k-th NN	$d(f, f(\mathcal{N}_k))$	d_k
LDOF	$\frac{\bar{d}}{\bar{D}}$	
Global FRE	$\ f - \hat{\tau}(\tau(f))\ _2$, where τ , is the forward PCA transformation, and $\hat{\tau}$ is its Moore-Penrose pseudo-inverse	
Class FRE	$\ f - \hat{\tau}_c(\tau_c(f))\ _2$ where τ_c is the PCA model for the class predicted by p	
Max(linear)	$\max(p)$	
Max(knn)	$\max(p_{\mathcal{N}})$	
Max(linear-T-scaled)	$\max(p_{2.0})$	
Max(linear+kNN)	$\max((p + p_{\mathcal{N}})/2)$	
TD(linear, kNN)	See Figure 5	TD
Entropy of NN's true class	$H(p_{\mathcal{N}})$	$H_{\mathcal{N}}$
EnWeDi(1st)	$d_1 \cdot (1 + H_{\mathcal{N}})$	
EnWeDi(average)	$\bar{d} \cdot (1 + H_{\mathcal{N}})$	
Feature entropy	$H(f/ f)$, where $ f $ defines the number of elements in f	
Feature sum	$\sum_a(f_a)$, where a indexes the feature elements	
Feature magnitude	$\ f\ _2$	
Avg. true probability of NN	$\frac{1}{k} \sum_n^k p_{c=\mathcal{T}(\mathcal{N}_n)}$, where $p_{c=\mathcal{T}(\mathcal{N}_n)}$ is the true class probability for \mathcal{N}_n	

Table 7. Mathematical definitions of OOD measures. See Table 6 for basic definitions

8.3. Effect of reference

Classifier definition	Exclude incorrect from ROC	ROC truth	Multi-class score	AUROC	TPR @1%FPR	% ID-incorrect* rejected	% ID-incorrect* - min	OOD vs ID-incorrect* accuracy	OOD vs ID-incorrect* F1
ID-correct vs rest	no	ID vs OOD	ID	98.2	78	9.8	9.8	-	-
Multi-class	no	not(ID-correct)	ID	97	78.9	8	8	-	-
ID vs OOD	no	not(ID-correct)	ID	96.9	79.6	7.7	7.7	-	-
Multi-class	no	ID vs OOD	ID-correct	98.2	79.7	9.9	3.2	99.3	83.8
ID-correct vs rest	no	not(ID-correct)	ID	98.4	80.6	27.4	27.4	-	-
Multi-class	no	not(ID-correct)	ID-correct	98.4	81	26.6	7.3	98.4	85.8
ID vs OOD	no	ID vs OOD	ID	98.7	84.4	5.4	5.4	-	-
Multi-class	no	ID vs OOD	ID	98.7	84.6	5.8	5.8	-	-
ID-correct vs rest	yes	not(ID-correct)	ID	98.8	86.5	27.4	27.4	-	-
ID-correct vs rest	yes	ID vs OOD	ID	98.8	86.5	27.4	27.4	-	-
Multi-class	yes	not(ID-correct)	ID-correct	98.8	87	26.6	7.3	98.4	85.8
Multi-class	yes	ID vs OOD	ID-correct	98.8	87	26.6	7.3	98.4	85.8
Multi-class	yes	not(ID-correct)	ID	98.9	87	8	8	-	-
Multi-class	yes	ID vs OOD	ID	98.9	87	8	8	-	-
ID vs OOD	yes	not(ID-correct)	ID	98.9	87.4	7.6	7.6	-	-
ID vs OOD	yes	ID vs OOD	ID	98.9	87.4	7.6	7.6	-	-

Table 8. Effect of reference: MSM top-level

Classifier definition	Exclude incorrect from ROC	ROC truth		Multi-class score	AUROC	TPR @1%FPR	% ID-incorrect* rejected	% ID-incorrect* - min	OOD vs ID-incorrect* accuracy	OOD vs ID-incorrect* F1
Multi-class	no	ID OOD	vs	ID	98.8	67.4	5.6	5.6	-	-
ID vs OOD	no	ID OOD	vs	ID	98.7	68	6	6	-	-
Multi-class	no	ID OOD	vs	ID-correct	98.4	70.6	5.4	4.9	98.5	53.7
ID-correct vs rest	no	ID OOD	vs	ID	98.3	70.6	6	6	-	-
ID-correct vs rest	no	not(ID-correct)		ID	98.4	83.6	24.2	24.2	-	-
Multi-class	no	not(ID-correct)		ID	97.5	83.7	20.7	20.7	-	-
ID vs OOD	no	not(ID-correct)		ID	97.3	84	20.7	20.7	-	-
Multi-class	no	not(ID-correct)		ID-correct	98.4	84.1	24.1	21.5	96.2	54.4
ID-correct vs rest	yes	not(ID-correct)		ID	99.5	92.6	24.2	24.2	-	-
ID-correct vs rest	yes	ID OOD	vs	ID	99.5	92.6	24.2	24.2	-	-
Multi-class	yes	not(ID-correct)		ID-correct	99.5	93.2	24.1	21.5	96.2	54.4
Multi-class	yes	ID OOD	vs	ID-correct	99.5	93.2	24.1	21.5	96.2	54.4
Multi-class	yes	not(ID-correct)		ID	99.6	93.3	20.7	20.7	-	-
Multi-class	yes	ID OOD	vs	ID	99.6	93.3	20.7	20.7	-	-
ID vs OOD	yes	not(ID-correct)		ID	99.6	93.6	20.7	20.7	-	-
ID vs OOD	yes	ID OOD	vs	ID	99.6	93.6	20.7	20.7	-	-

Table 9. Effect of reference: MSM Norwegian vertebrates

Classifier definition	Exclude incorrect from ROC	ROC truth	Multi-class score	AUROC	TPR @1%FPR	% ID-incorrect* rejected	% ID-incorrect* rejected - min	OOD vs ID-incorrect* accuracy	OOD vs ID-incorrect* F1
ID-correct vs rest	no	ID vs OOD	ID	96.3	58.5	0	0	-	-
Multi-class	no	ID vs OOD	ID-correct	96.4	58.6	0	0	-	-
ID-correct vs rest	no	not(ID-correct)	ID	95.5	66.7	10.7	10.7	-	-
ID vs OOD	no	not(ID-correct)	ID	92.3	67.3	7.8	7.8	-	-
Multi-class	no	not(ID-correct)	ID	92.9	68.2	8.8	8.8	-	-
ID vs OOD	no	ID vs OOD	ID	98	68.9	2	2	-	-
Multi-class	no	not(ID-correct)	ID-correct	95.5	69.1	12.7	8.9	95.9	64.1
Multi-class	no	ID vs OOD	ID	98	70.3	2.2	2.2	-	-
ID-correct vs rest	yes	not(ID-correct)	ID	98.9	85.4	10.7	10.7	-	-
ID-correct vs rest	yes	ID vs OOD	ID	98.9	85.4	10.7	10.7	-	-
ID vs OOD	yes	not(ID-correct)	ID	99.2	87.7	7.8	7.8	-	-
ID vs OOD	yes	ID vs OOD	ID	99.2	87.7	7.8	7.8	-	-
Multi-class	yes	not(ID-correct)	ID-correct	98.8	87.9	12.7	8.9	95.9	64.1
Multi-class	yes	ID vs OOD	ID-correct	98.8	87.9	12.7	8.9	95.9	64.1
Multi-class	yes	not(ID-correct)	ID	99.2	88.5	8.8	8.8	-	-
Multi-class	yes	ID vs OOD	ID	99.2	88.5	8.8	8.8	-	-

Table 10. Effect of reference: : iNaturalist 2018

8.4. SHAP analysis

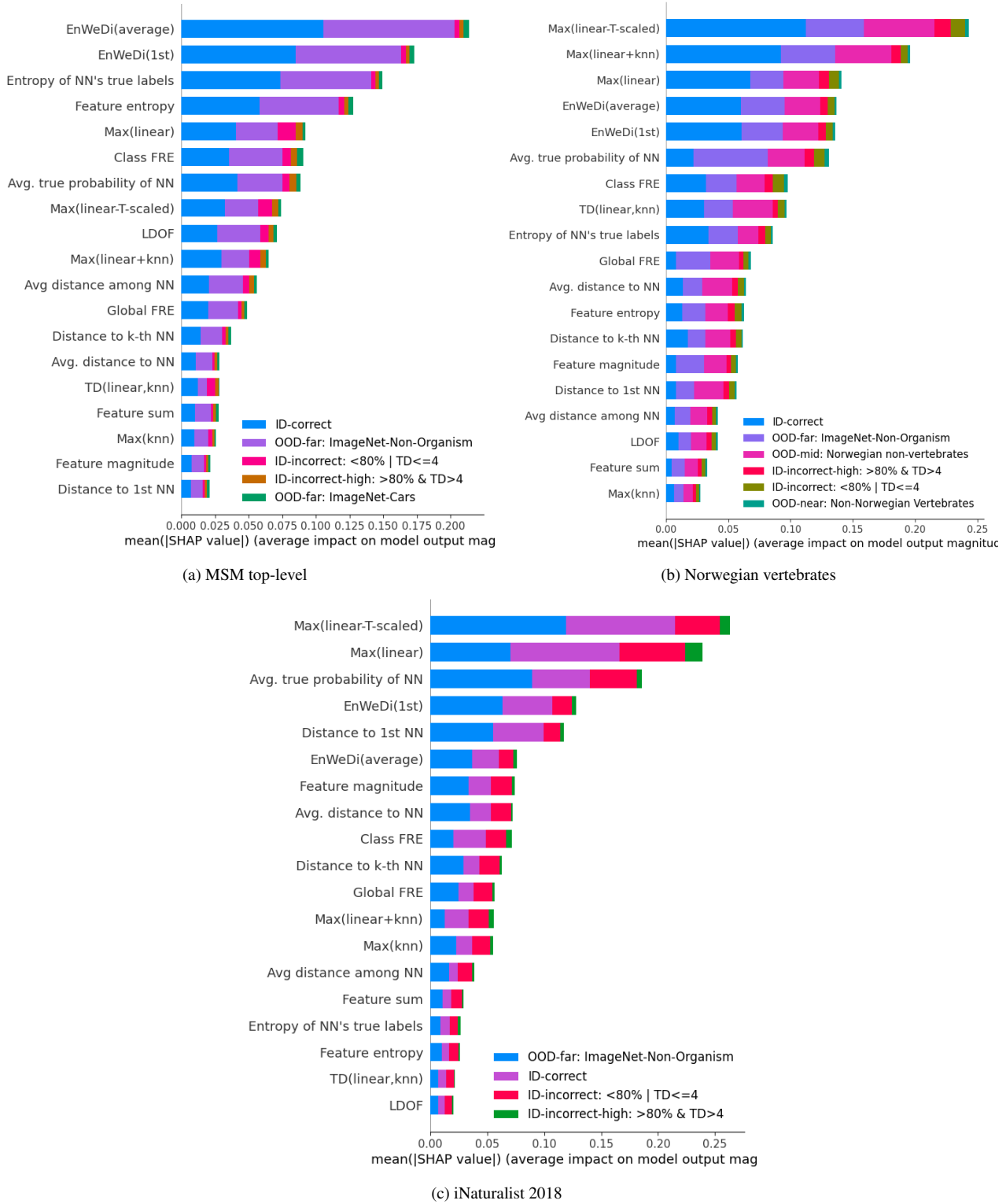


Figure 6. SHAP analysis showing individual OOD measures most contributing to the COOD model

8.4.1 SHAP analysis per output category

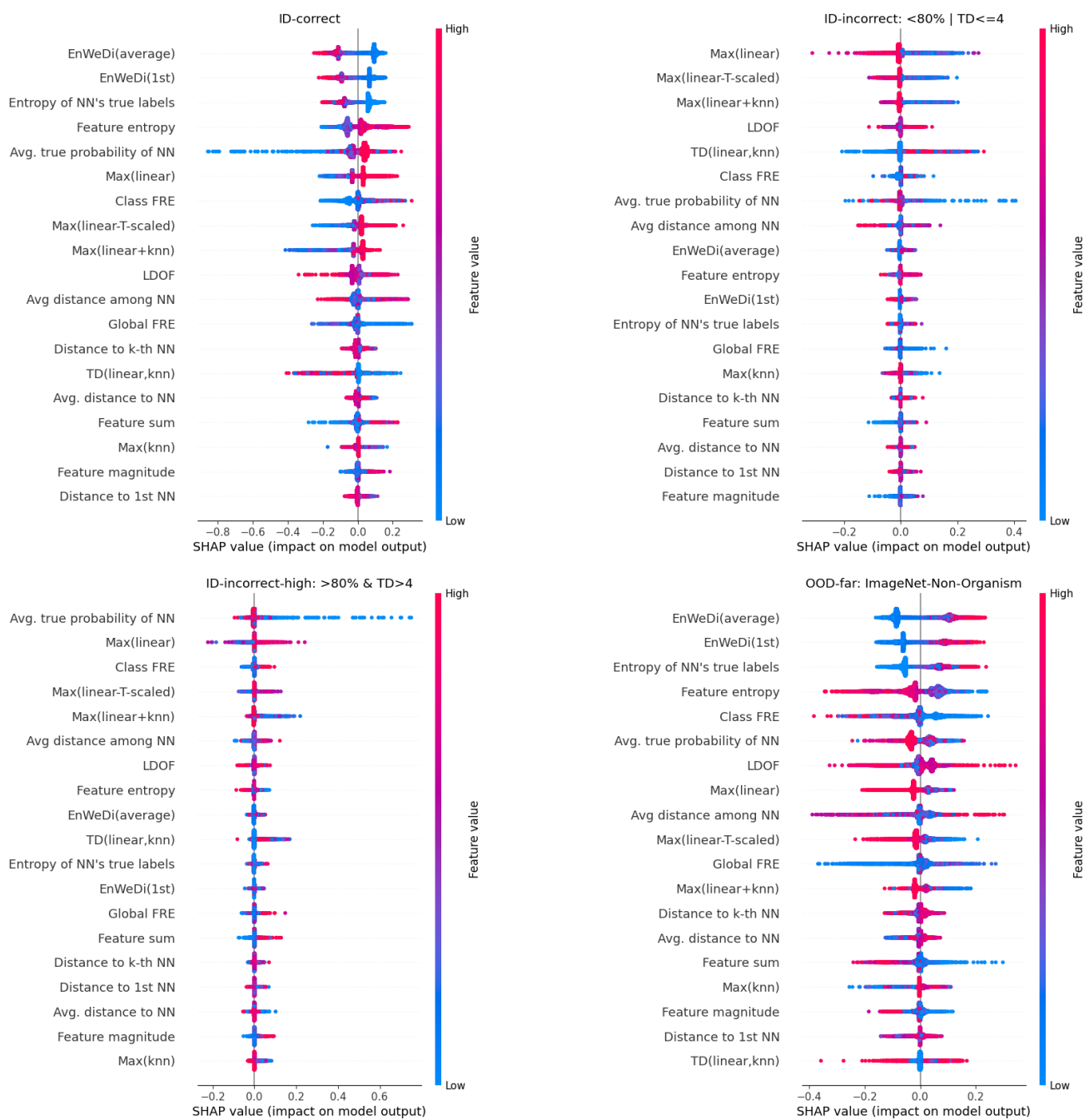


Figure 7. SHAP analysis per output category: MSM top-level

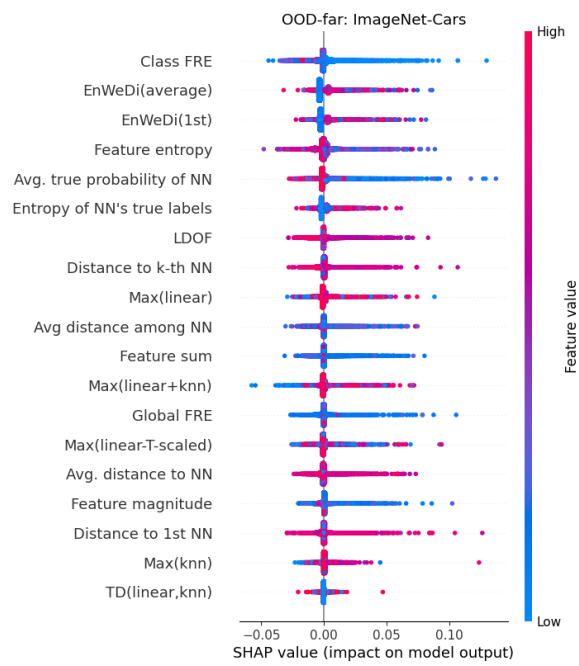


Figure 7. SHAP analysis per output category: MSM top-level (cont.)

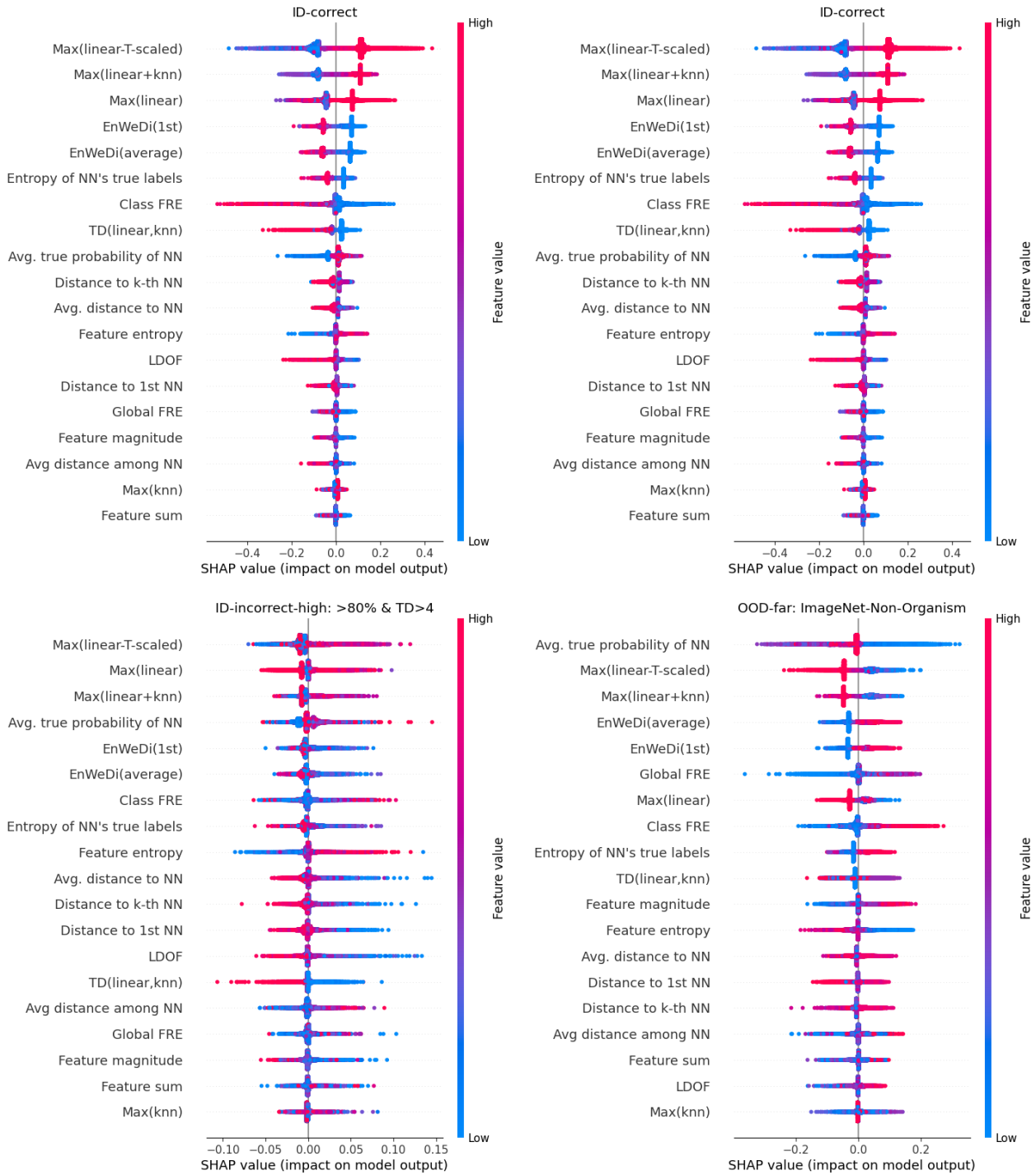


Figure 8. SHAP analysis per output category: Norwegian vertebrates

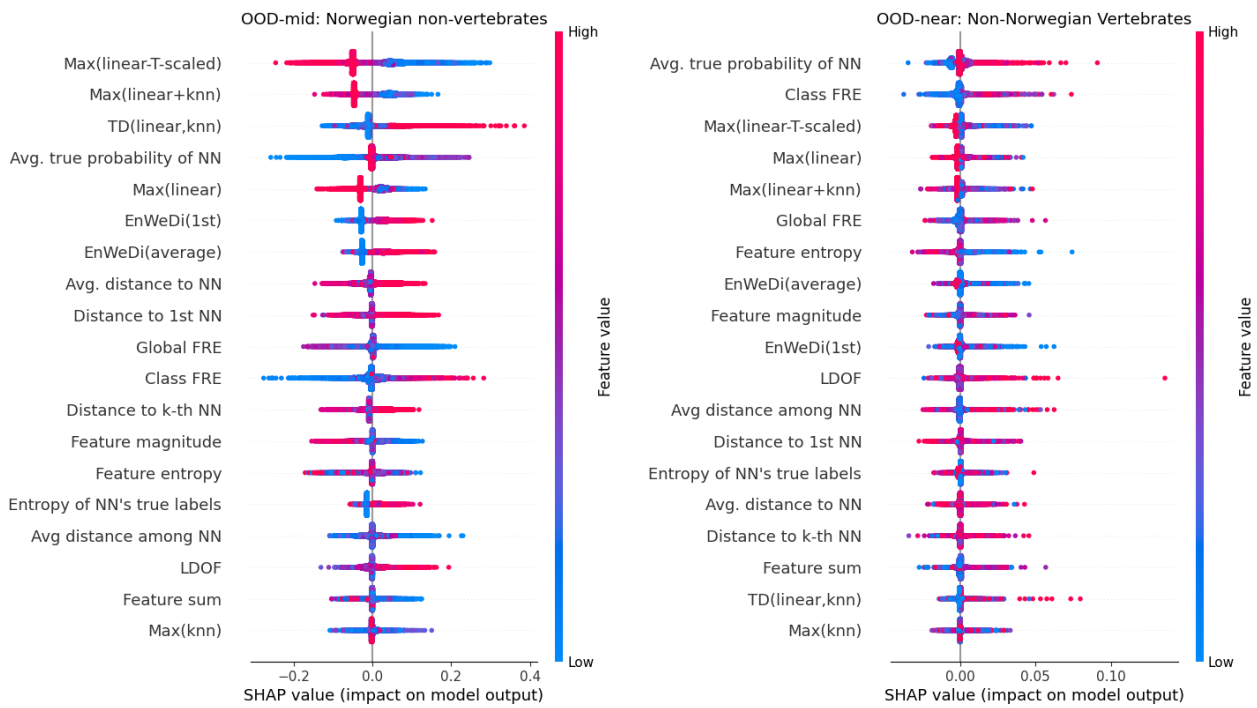


Figure 8. SHAP analysis per output category: Norwegian vertebrates (cont.)

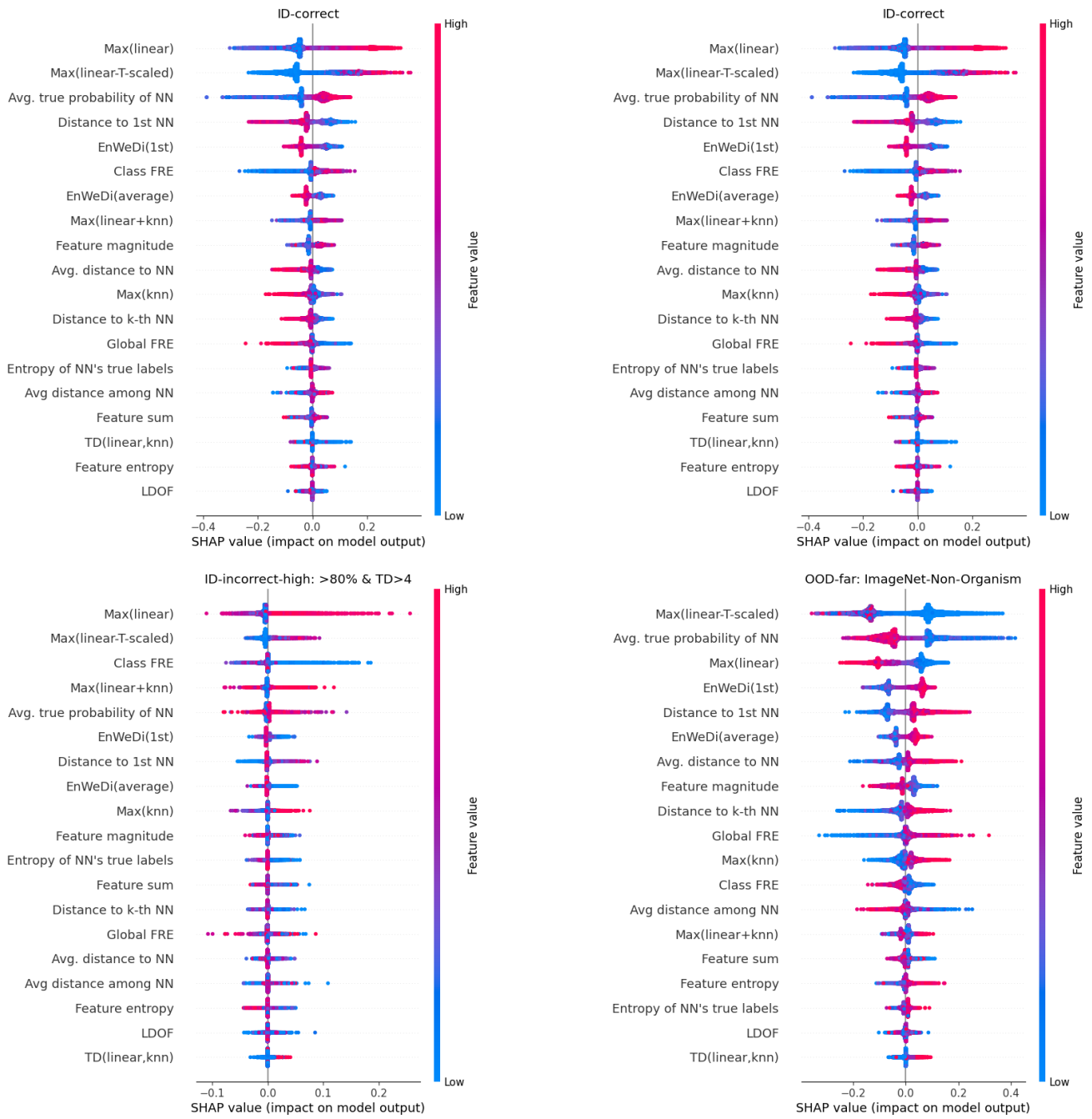


Figure 9. SHAP analysis per output category: iNaturalist 2018

8.5. COOD score distribution and ROC analysis

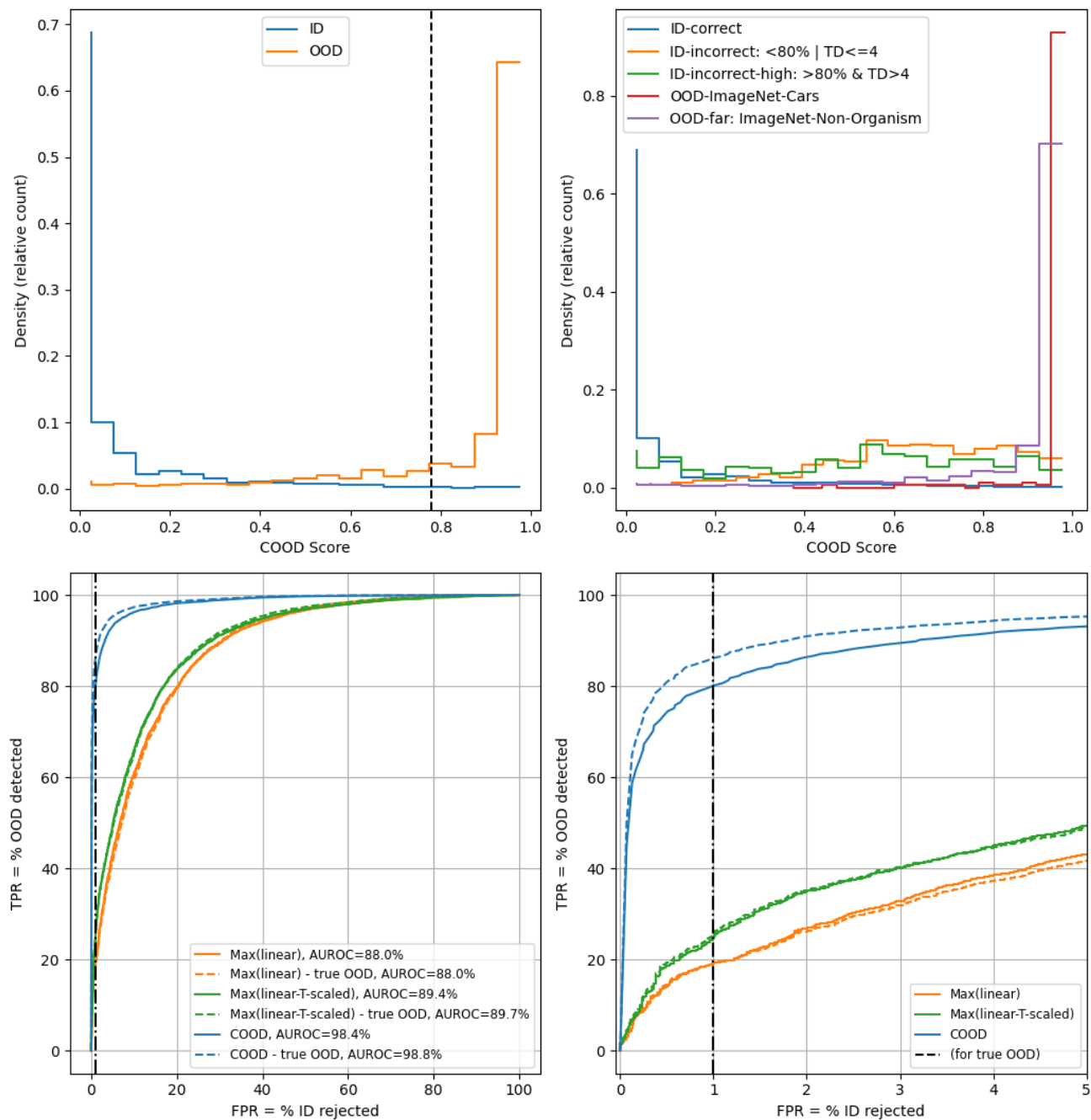


Figure 10. COOD score distribution and ROC analysis for MSM top-level

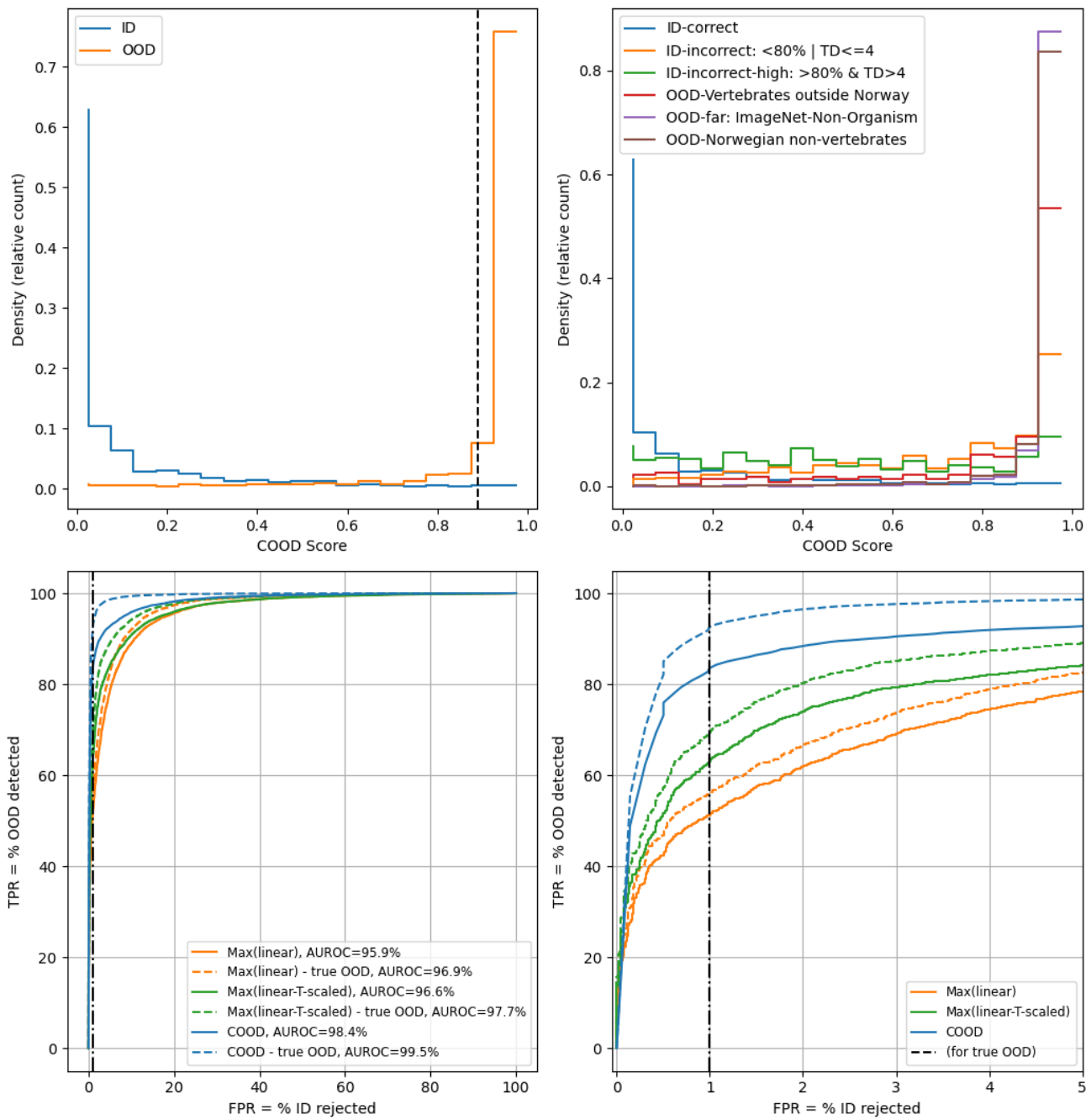


Figure 11. COOD score distribution and ROC analysis for Norwegian vertebrates

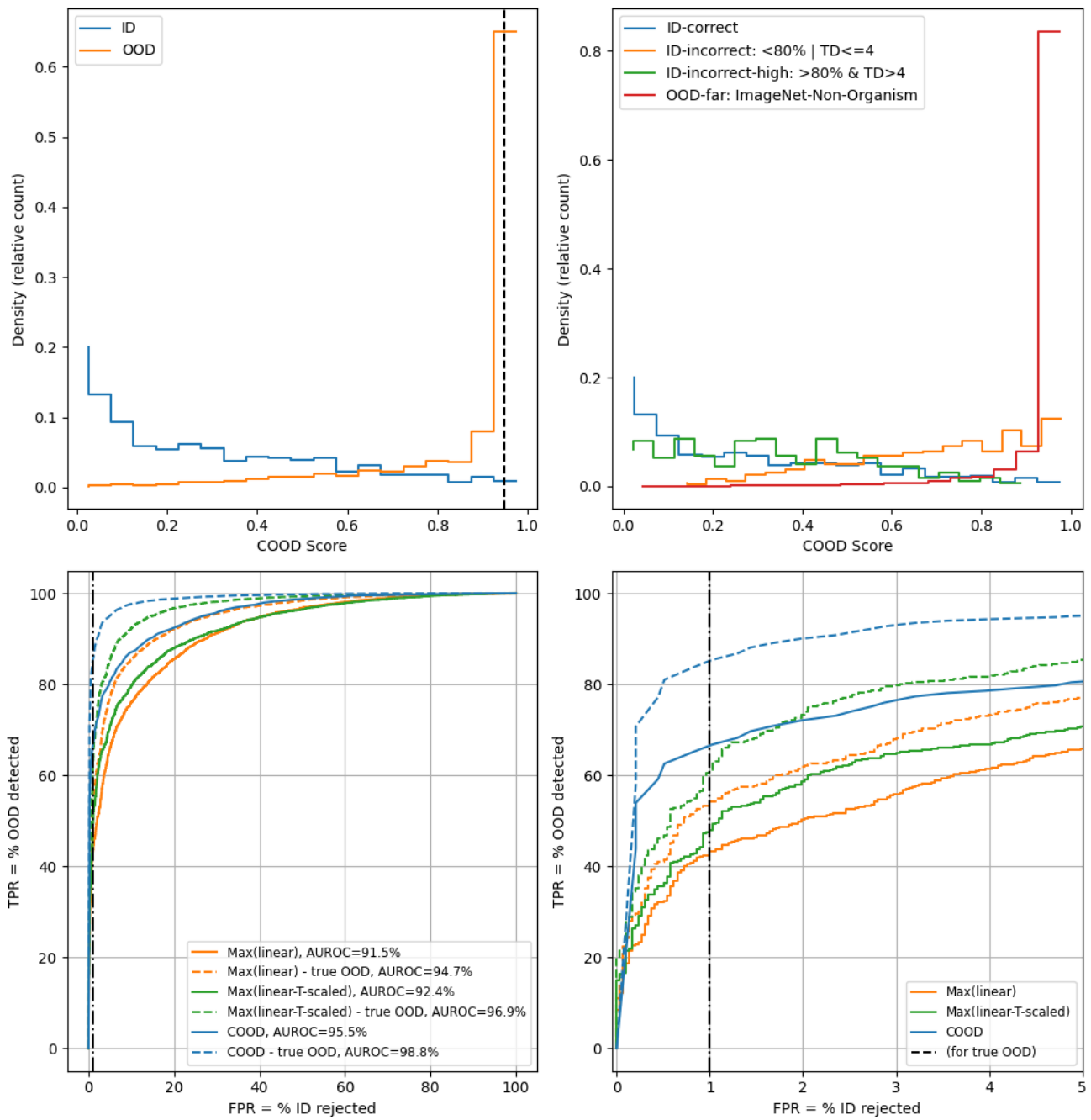
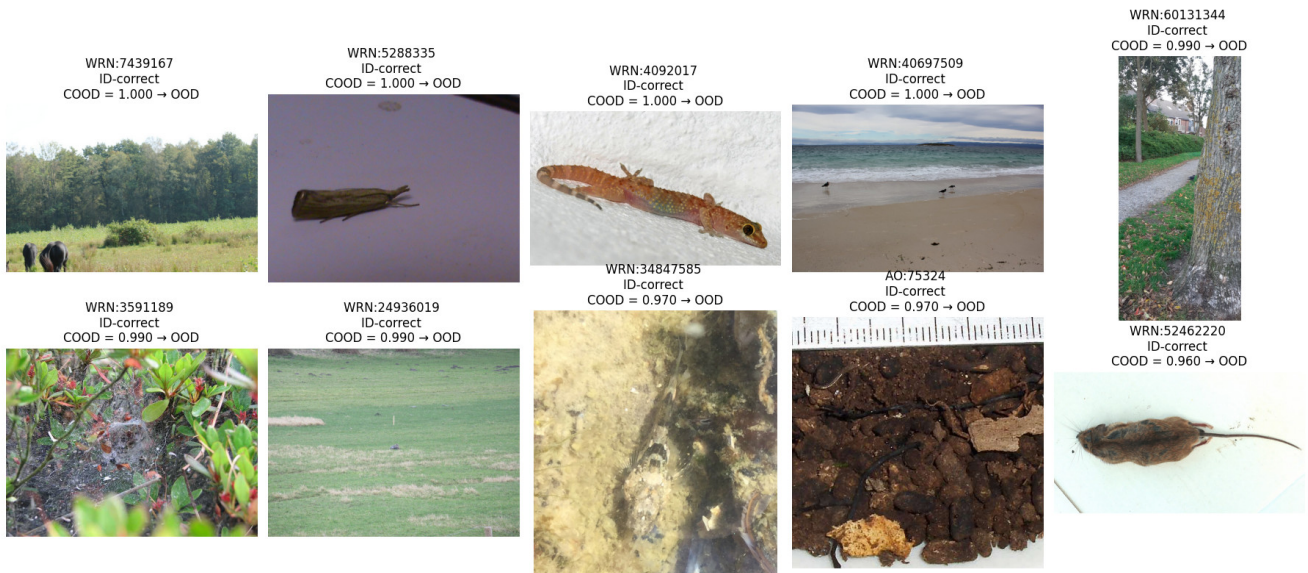


Figure 12. COOD score distribution and ROC analysis for iNaturalist 2018

8.6. Example images

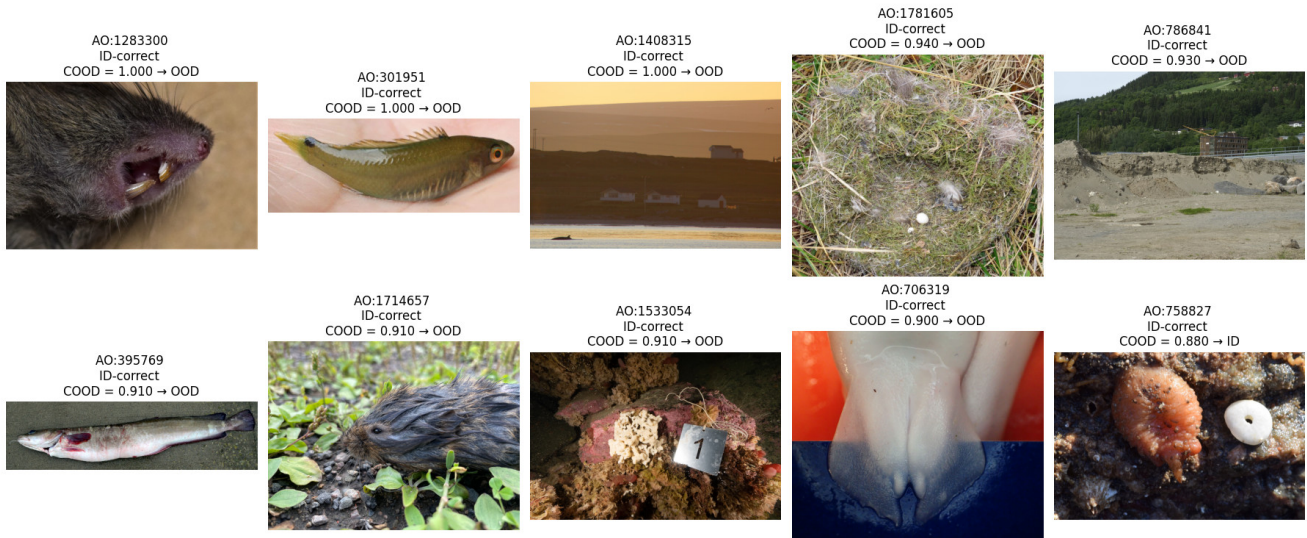


(a) False positives (high COOD score for ID images)



(b) False negatives (low COOD score for OOD images)

Figure 13. Selected examples of MSM top-level



(a) False positives (high COOD score for ID images)



(b) False negatives (low COOD score for OOD images)

Figure 14. Selected examples of Norwegian vertebrates

8.7. Visual example licences

uid	author	date	license	image_url
WRN:7439167	Ted van der Knaap	2014-09-18	CC BY-NC-ND	waarneming.nl/photos/7439167
WRN:60131344	Jona Haasnoot	2022-10-24	CC BY-NC-ND	waarneming.nl/photos/60131344
WRN:24936019	Theo Ruppert	2020-02-20	CC BY-NC-ND	waarneming.nl/photos/24936019
WRN:40697509	KJ Hijlkema	2018-03-12	CC BY-NC-ND	waarneming.nl/photos/40697509
WRN:4092017	Harm Alberts	2012-10-01	CC BY-NC-ND	waarneming.nl/photos/4092017
WRN:3591189	Veerle De Saedeleer	2012-07-07	CC BY-NC-ND	waarneming.nl/photos/3591189
WRN:5288335	Ruben Vernieuwe	2013-08-09	CC BY-NC-ND	waarneming.nl/photos/5288335
WRN:34847585	Jeroen Hoek	2021-04-28	CC BY-NC-ND	waarneming.nl/photos/34847585
AO:75324	Magne Flåten	2008-06-17	CC BY-SA	artsobservasjoner.no/Image/75324
WRN:52462220	Cor de Jong	2022-06-20	CC BY-NC-ND	waarneming.nl/photos/52462220

Table 11. MSM top-level: License information for visual examples

uid	author	date	license	image_url
AO:301951	Magne Flåten	2012-02-09	CC BY-SA	artsobservasjoner.no/Image/301951
AO:1408315	Karel Samyn	2020-07-13	CC BY-NC-SA	artsobservasjoner.no/Image/1408315
WRN:1587318	Frans Rosmalen	2010-09-24	CC BY-NC-ND	waarneming.nl/photos/1587318
WRN:8530324	Paul Schrijvershof	2015-03-22	CC BY-NC	waarneming.nl/photos/8530324
WRN:41208597	Jos Cuppens	2021-08-14	CC BY-NC-ND	waarneming.nl/photos/41208597
WRN:22944939	David Tempelman	2019-08-25	CC0	waarneming.nl/photos/22944939
WRN:20030511	Frens Westenbrink	2019-03-31	CC BY-NC-ND	waarneming.nl/photos/20030511
AO:1283300	Johan Sirnes	2020-01-17	CC BY	artsobservasjoner.no/Image/1283300
WRN:16133685	Hans Verdaat	2018-01-21	CC BY-NC-ND	waarneming.nl/photos/16133685
AO:1714657	Eric Francois Roualet	2021-06-08	CC BY-NC-SA	artsobservasjoner.no/Image/1714657
AO:395769	Kristoffer Bøhn	2014-01-03	CC BY-NC-SA	artsobservasjoner.no/Image/395769
AO:1781605	Magne Flåten	2013-12-09	CC BY-SA	artsobservasjoner.no/Image/1781605
AO:1533054	Ole Meldahl	2020-12-26	CC BY-SA	artsobservasjoner.no/Image/1533054
AO:706319	Magne Flåten	2016-11-29	CC BY-SA	artsobservasjoner.no/Image/706319
AO:786841	Anders Breili	2017-06-17	CC BY-NC-SA	artsobservasjoner.no/Image/786841
AO:758827	Johan Sirnes	2017-04-29	CC BY	artsobservasjoner.no/Image/758827

Table 12. Norwegian vertebrates: License information for visual examples