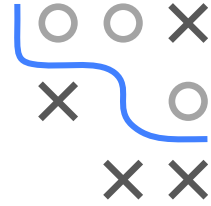
Introduction to Machine Learning

Evaluation
Multi-Class AUC



AUC(pos|neg) = AUC(1|3)

	Y	$\hat{\pi}_1$	$\hat{\pi}_2$	$\hat{\pi}_3$
pos	1	0.7	0.2	0.1
pos	1	0.5	0.3	0.2
~~pos~~	~~2~~	~~0.3~~	~~0.5~~	~~0.2~~
~~pos~~	~~2~~	~~0.4~~	~~0.5~~	~~0.1~~
neg	3	0.6	0.1	0.3
neg	3	0.1	0.1	0.8

AUC(pos|neg) = AUC(3|1)

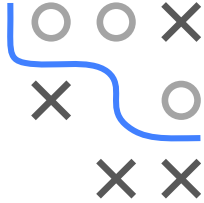
	Y	$\hat{\pi}_1$	$\hat{\pi}_2$	$\hat{\pi}_3$
neg	1	0.7	0.2	0.1
neg	1	0.5	0.3	0.2
~~neg~~	~~2~~	~~0.3~~	~~0.5~~	~~0.2~~
~~neg~~	~~2~~	~~0.4~~	~~0.5~~	~~0.1~~
pos	3	0.6	0.1	0.3
pos	3	0.1	0.1	0.8

Learning goals

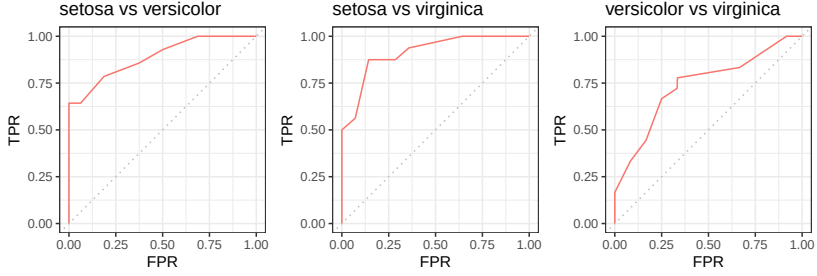
- Understand that generalizing AUC to multi-class is not trivial
- Learn how multi-class AUC can be derived

MULTI-CLASS AUC

- AUC and other ROC metrics for binary classification
- Different ways to estimate **multi-class AUC**
- Often based on aggregated binary AUCs:
  e.g. 1-vs-1 or 1-vs-rest

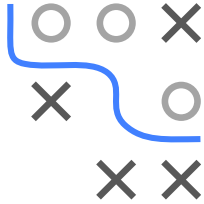


Example: 1-vs-1 on `iris`



MULTI-CLASS AUC

- Def AUC($k \mid \ell$) for classes k (pos) and ℓ (neg)
- Compute AUC: Subset preds to rows of true k and ℓ, use $\hat{\pi}_k$
- Interprete: Prob that random member of ℓ has a lower prob to belong to class k than random member of class k.



Example: AUC(3|1) with $g = 3$ classes

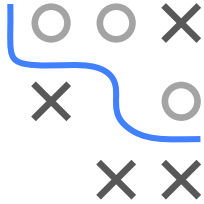
AUC(pos|neg) = AUC(3|1)

	Y	$\hat{\pi}_1$	$\hat{\pi}_2$	$\hat{\pi}_3$
neg	1	0.7	0.2	0.1
neg	1	0.5	0.3	0.2
	2	0.3	0.5	0.2
	2	0.4	0.5	0.1
pos	3	0.6	0.1	0.3
pos	3	0.1	0.1	0.8

1. Subset pred rows to true classes 1 and 3
2. Use $k = 3$ as pos and $\ell = 1$ as neg class
3. Compute standard AUC with $\hat{\pi}_3$ as scores
4. AUC(3|1) = 1:
   all pos have higher $\hat{\pi}_3$ than negs

MULTI-CLASS AUC

- For binary classes: always $\text{AUC}(1|0) = \text{AUC}(0|1)$
- For multi-class usually: $\text{AUC}(k \mid \ell) \neq \text{AUC}(\ell \mid k)$
- **Example** with $g = 3$ where $\text{AUC}(1|3) \neq \text{AUC}(3|1)$:
  - $\text{AUC}(3|1) = 1$ (RHS) as before
  - $\text{AUC}(1|3) \neq 1$ (LHS)



AUC(pos|neg) = AUC(1|3)

	Y	$\hat{\pi}_1$	$\hat{\pi}_2$	$\hat{\pi}_3$
pos	1	0.7	0.2	0.1
pos	1	0.5	0.3	0.2
	2	0.3	0.5	0.2
	2	0.4	0.5	0.1
neg	3	0.6	0.1	0.3
neg	3	0.1	0.1	0.8

AUC(pos|neg) = AUC(3|1)

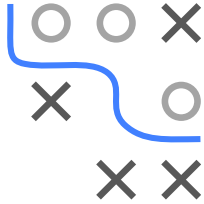
	Y	$\hat{\pi}_1$	$\hat{\pi}_2$	$\hat{\pi}_3$
neg	1	0.7	0.2	0.1
neg	1	0.5	0.3	0.2
	2	0.3	0.5	0.2
	2	0.4	0.5	0.1
pos	3	0.6	0.1	0.3
pos	3	0.1	0.1	0.8

MULTI-CLASS AUC

Hand and Till (2001) proposed to avg AUC via **1-vs-1**:

- For all class pairs, compute AUC($k \mid \ell$).

$$\text{AUC}_{MC} = \frac{1}{g(g-1)} \sum_{k \neq \ell} \text{AUC}(k|\ell) \in [0, 1].$$



Comments:

- Other defs use **1-vs-rest** and need to avg only g AUC values
- 1-vs-rest creates imbal classes even if orig classes are balanced
- Imbalanced classes can be considered by weighting individual AUC values with class priors [Ferri et al. (2003)]