

Soft Classifiers

with continuous class membership $\in [0, 1]$ model

- uncertainty/probability
 - (dis)agreement of panel of pathologists
 - probability of sample belonging to class
- mixtures
 - samples between classes
 - e.g. currently undergoing de-differentiation
 - mixtures of cells

Soft prediction: common, e.g. posterior probabilities

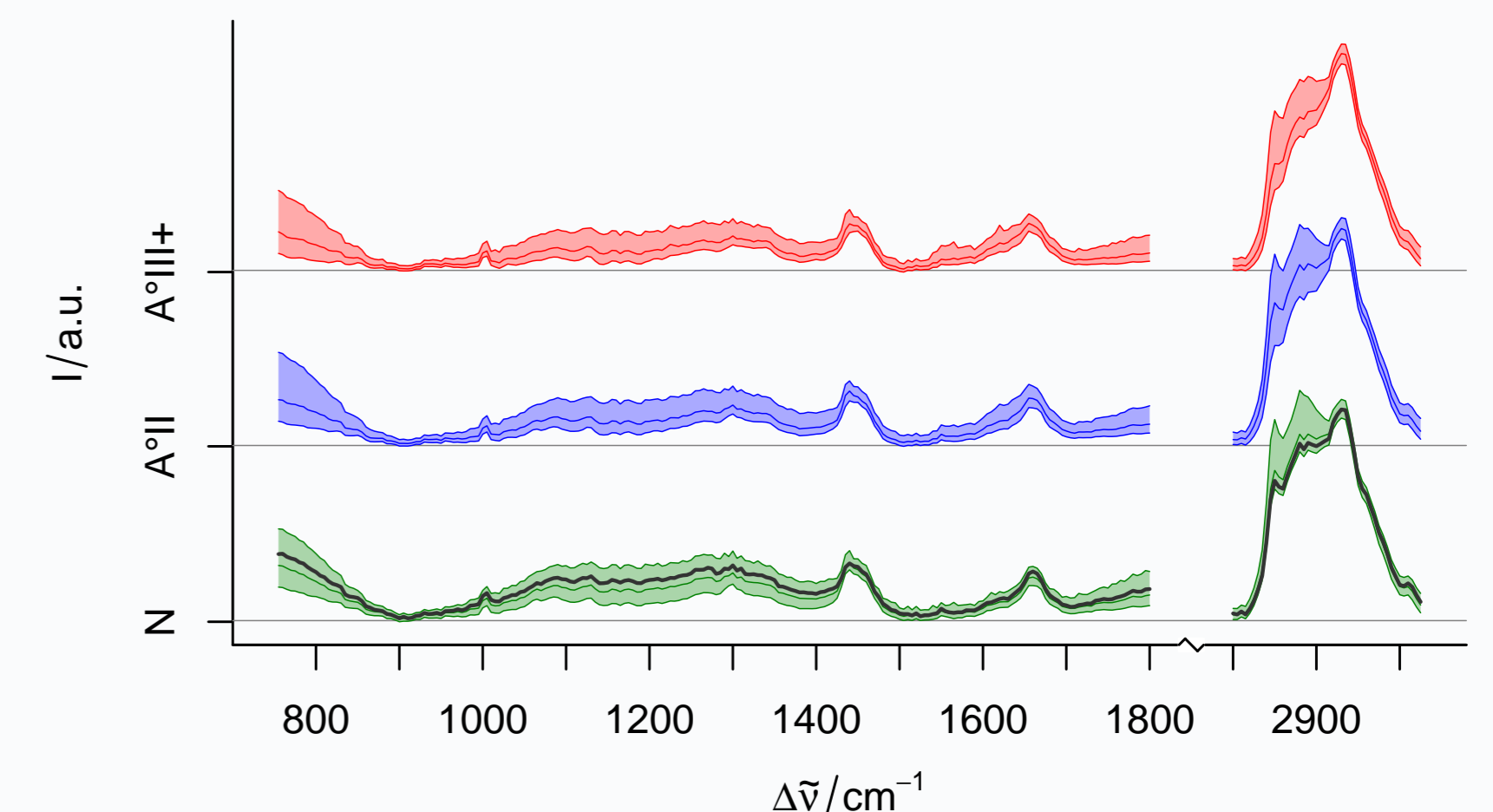
Soft training: available, e.g. Beleites *et. al.*, ABC, 400, 2801ff.

Soft validation: **needed**

borderline cases target of new diagnostics.

Example: Grading of Astrocytoma Tissues

class	crisp only		soft	
	patients	spectra	patients	spectra
Normal	16	7 456	35	15 747
thereof controls	9	4 902	9	4 902
Astrocytoma ^o II	17	4 171	47	19 128
Astrocytoma ^o III+	27	8 279	53	21 617
total	53	19 906	80	37 015



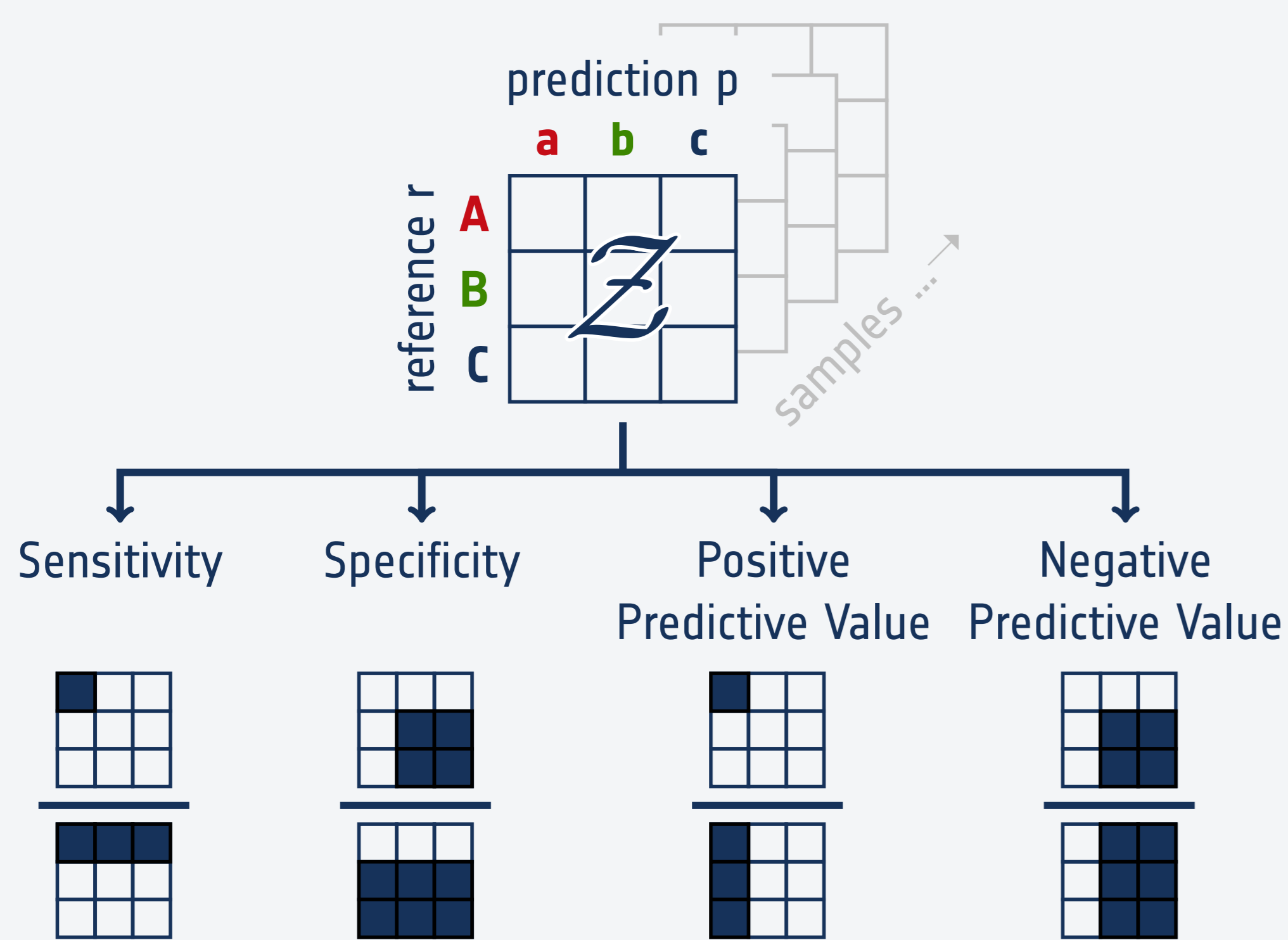
Aim: grading of ambiguous tissue regions

Data set: Raman maps of bulk samples in moist chamber

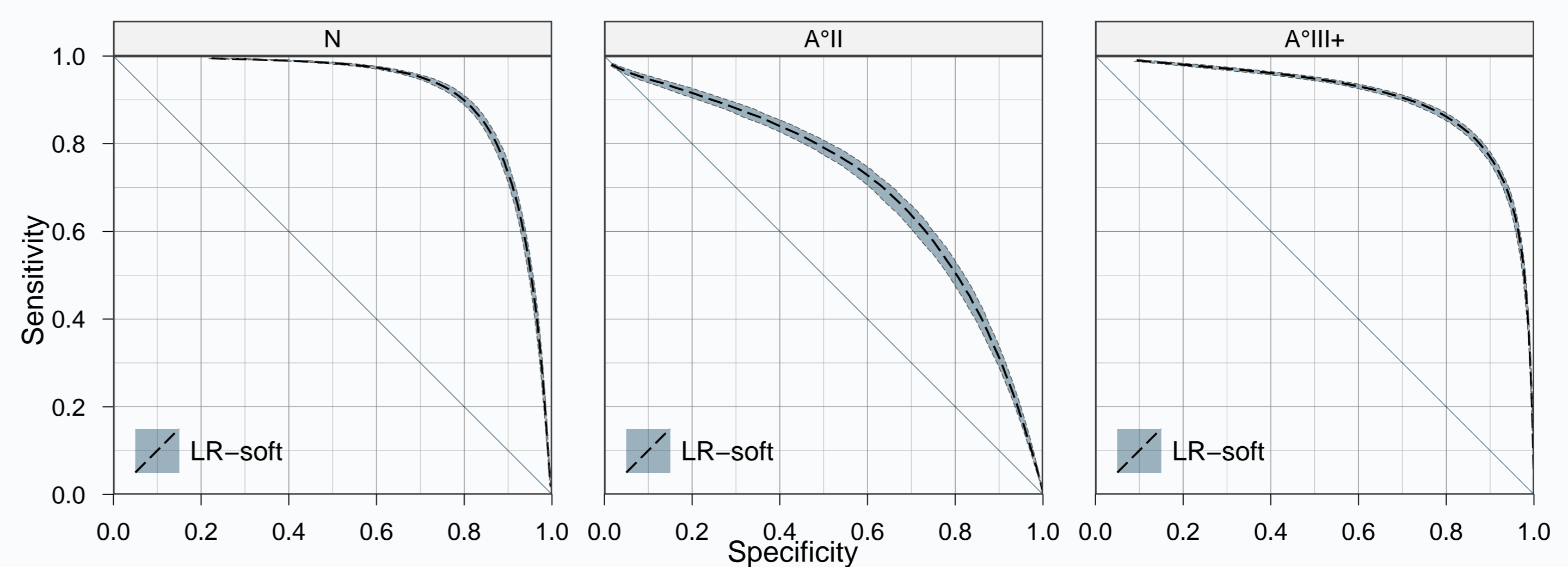
Classifier: logistic regression

Validation: 125 × 8-fold cross validation (patient-wise splitting)

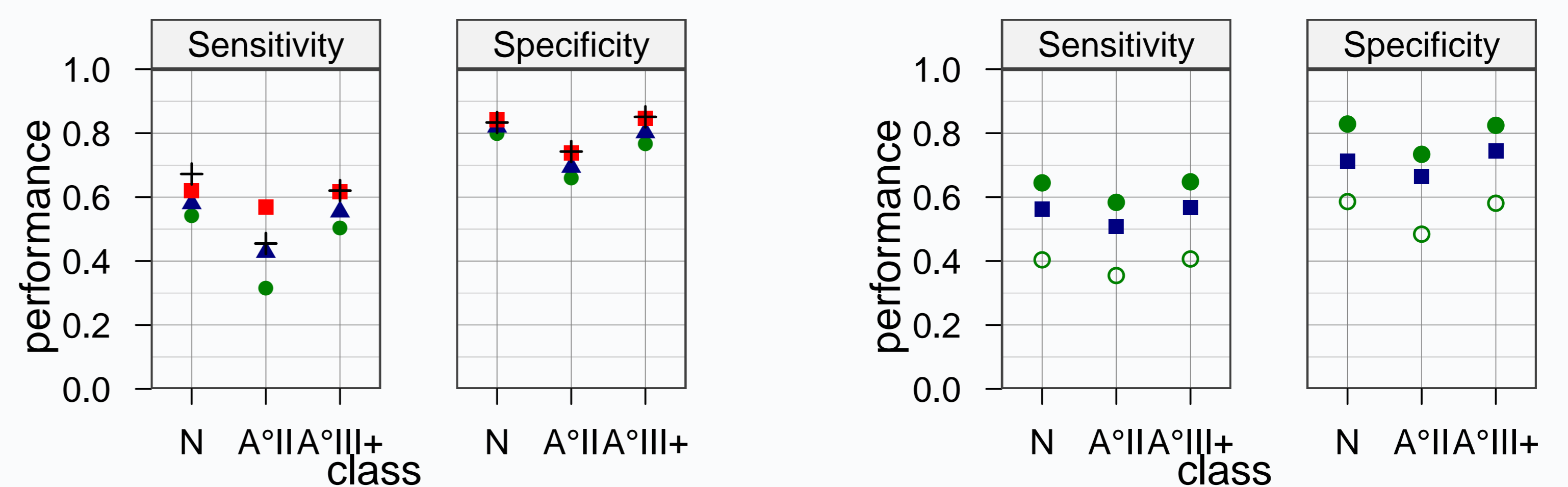
Classifier Performance Measures



Validation Results



Classical validation: "hardening" predictions of unambiguous samples



weak ■, product ▲, and strong ● AND. Unambiguous samples only +.

1 - wMAE ●, 1 - wRMSE ■, and lower bound of 1 - wRMSE, 1 - $\sqrt{\text{wMAE}}$ ○.

Soft validation:

- Soft performance more sensitive for slight errors than classical measures
- Many samples partially A^oII \rightsquigarrow large difference between weak and strong AND
- wRMSE close to wMAE: many samples with slight deviations

Soft Confusion Matrix Z

- for hard $r_i, p_j \in \{0, 1\}$ use classical AND: $Z_{i,j} = r_i \wedge p_j$
- generalizations for soft $r_i, p_j \in [0, 1]$

	strong AND	product AND	weak AND
$r_i = 0.5$			
$p_j = 0.8$			
$Z_{i,j} =$	$\max(r_i + p_j - 1, 0)$	$r_i \cdot p_j$	$\min(r_i, p_j)$
$=$	0.3	0.4	0.5
scenario	worst case	expected	best case

- calibration-like: weighted mean absolute error (wMAE) and weighted root mean square error (wRMSE)
- $$\text{wMAE} \leq \text{wRMSE} \leq \sqrt{\text{wMAE}}$$

Implementation

Implementation:  package `softclassval`

Homepage: `softclassval.r-forge.r-project.org`


License: GPL 3

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Conclusions

- Samples with partial class membership can be used for validation.
- For unambiguous samples, no hardening is required
- Soft performance more sensitive than classical hard performance
- Soft operators for worst case, best case, expected performance as well as calibration-type operators.
- Available as  package `softclassval`