

# Validation of Soft Classifiers for Cells and Tissues

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## 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

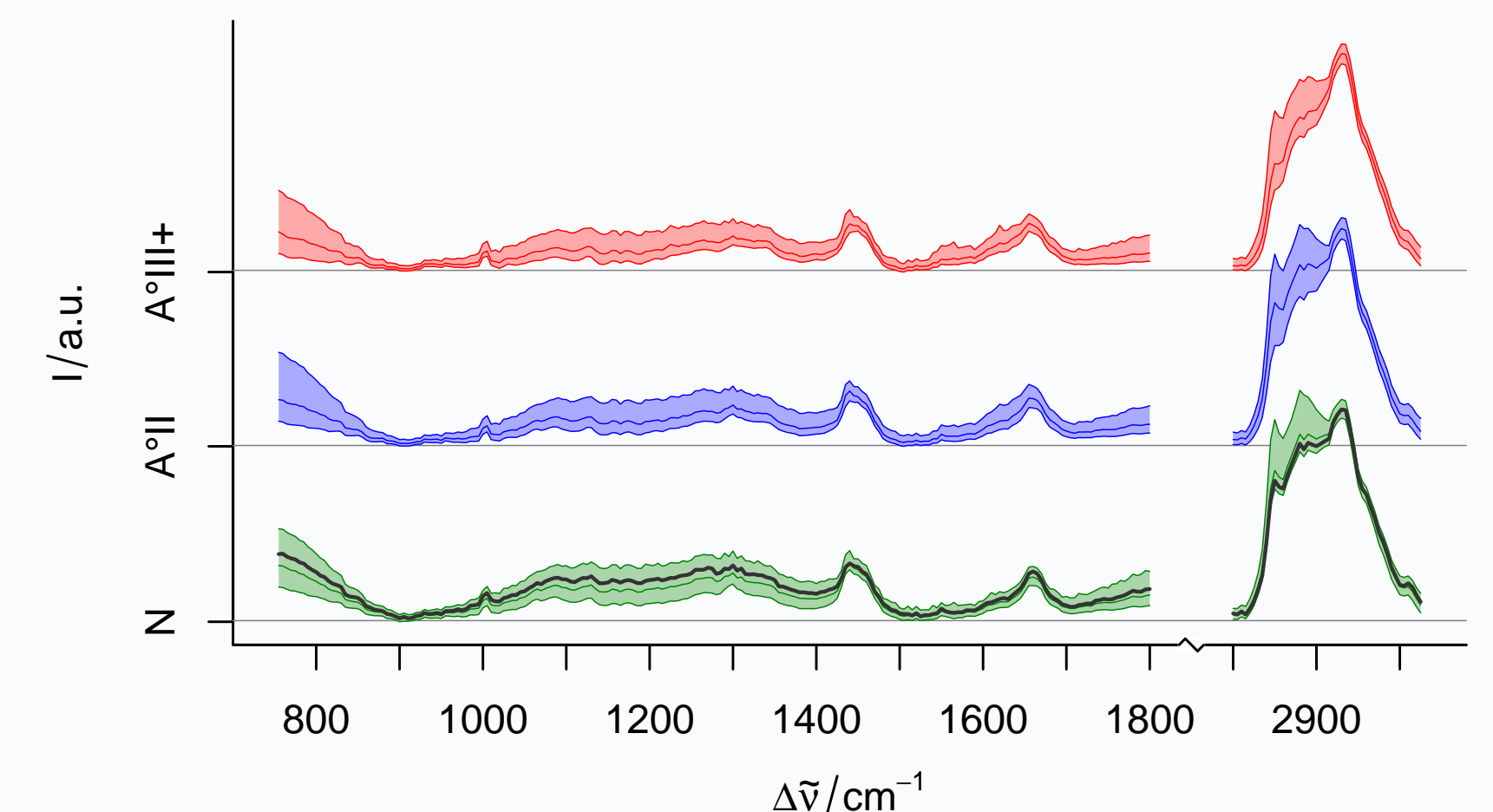
**Soft training:** available, e.g. Beleites *et. al.*, ABC, 400, 2801ff.

**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 <sup>o</sup> II	17	4 171	47	19 128
Astrocytoma <sup>o</sup> III+	27	8 279	53	21 617
total	53	19 906	80	37 015



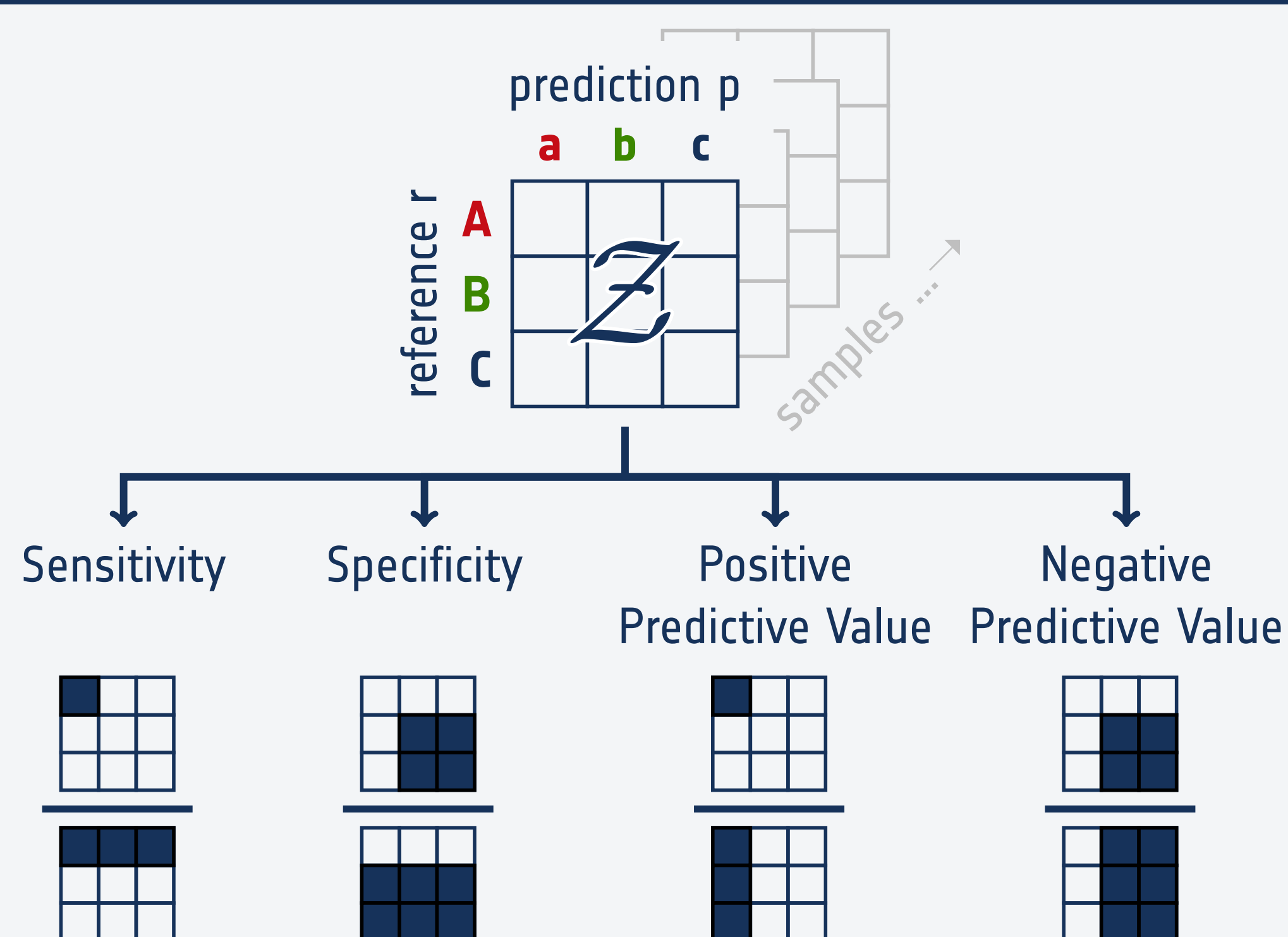
**Aim:** grading of ambiguous tissue regions

**Data set:** Raman maps of bulk samples in moist chamber

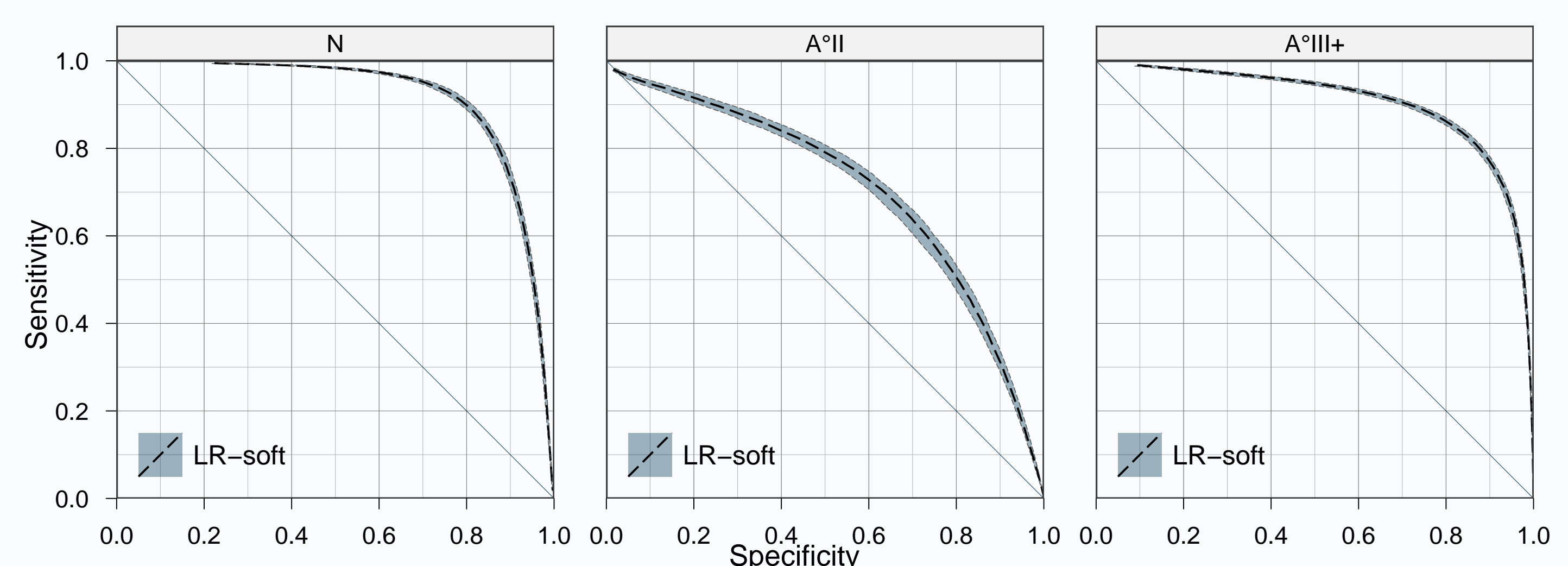
**Classifier:** logistic regression

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

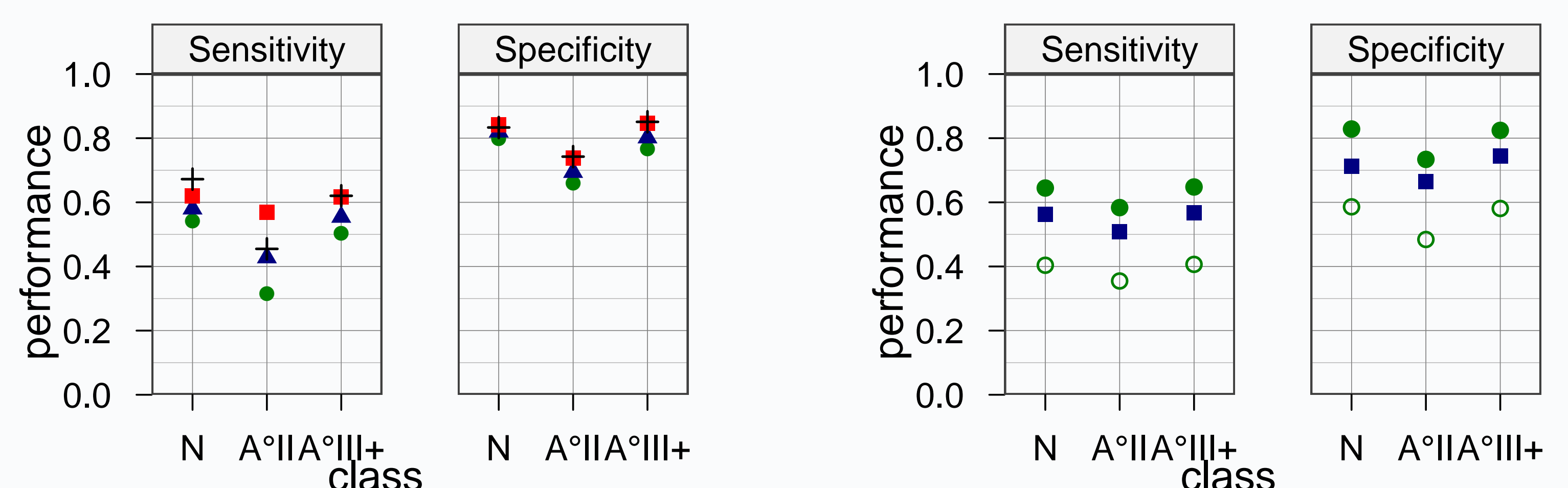
## Classifier Performance Measures



## 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 - √wMAE ○.

**Soft validation:**

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

## Soft Confusion Matrix $\mathcal{Z}$

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

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

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

## Implementation

**Implementation:**  package **softclassval**

**Homepage:** [softclassval.r-forge.r-project.org](https://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**