Bijective Transformation: Raw Spectrum → Categorical States

Raw Spectrum

Platform-Dependent

(m/z, intensity)

Example: 862 peaks

14D Feature Extraction

Feature Space

14D Coordinates

Structural (4D)
Statistical (4D)
Information (4D)
Temporal (2D)

S-Entropy Transform

S-Entropy Space

Platform-Independent

(S_k, S_t, S_e)

CV < 1%

Categorical Mapping

Categorical States

Discrete

Classes
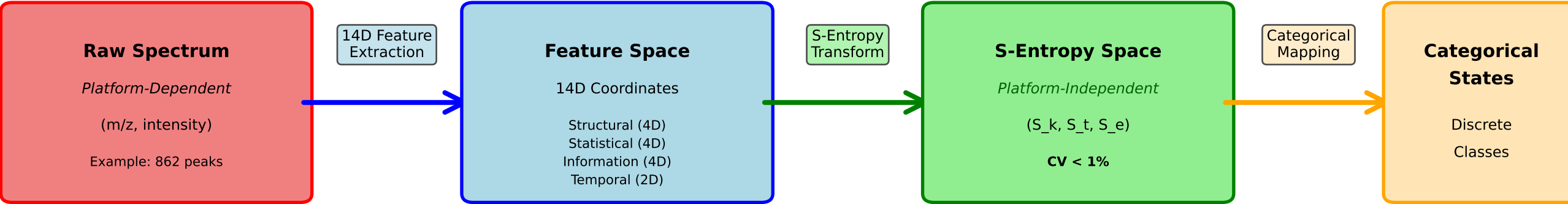
Inverse Transform (Reconstruction)

Bijective Properties:

1. Information Preservation

Reconstruction error $\varepsilon < 0.01$

Complete spectral recovery possible

2. Platform Independence

$||f(M\_A) - f(M\_B)||_2 < 0.01$

Same metabolite → same coordinates

3. Categorical Consistency

Lipid classes occupy distinct regions

Phase relationships preserved

$\Phi : M \mapsto \mathbf{f}(M)$ is bijective

Enables zero-shot transfer learning across platforms

Models trained on Platform A work directly on Platform B without retraining