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Beyond PCA: Robust Spectral Anomaly Detection in EELS-SI Using Deep Learning

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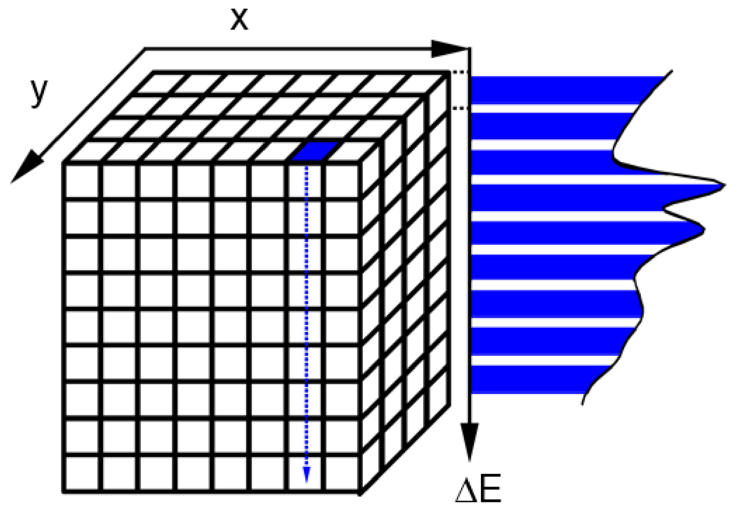
Introduction

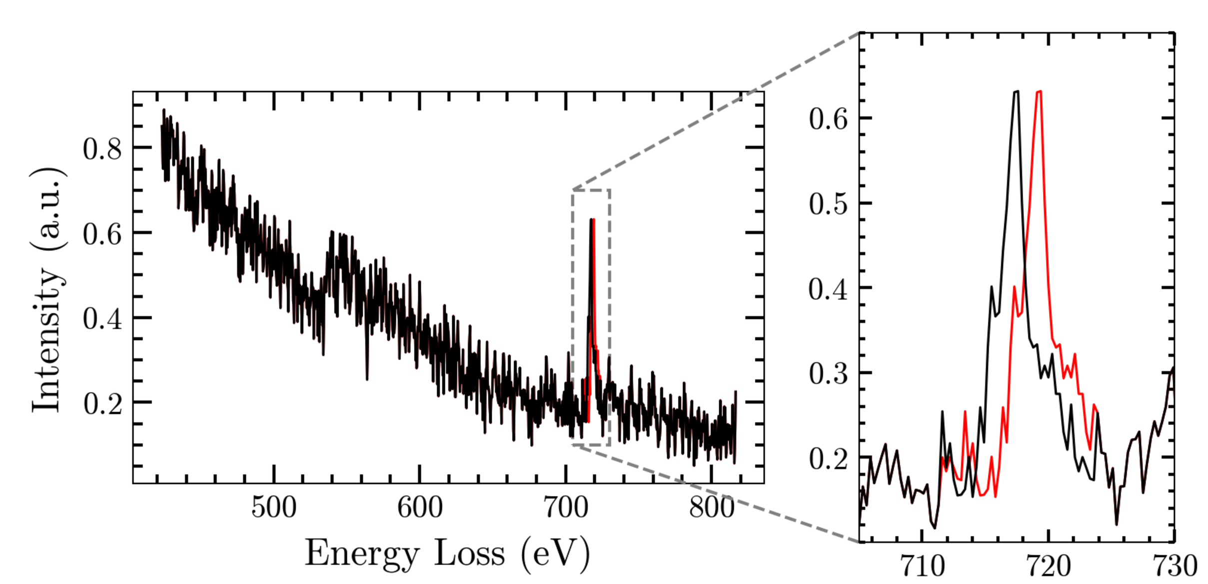
- Electron Energy Loss Spectroscopy with Spectrum Imaging (EELS-SI) measures the electronic structure of materials using inelastic electron scattering.
- Produces a spatial-resolved map at atomic resolution, creating a 3D data cube.



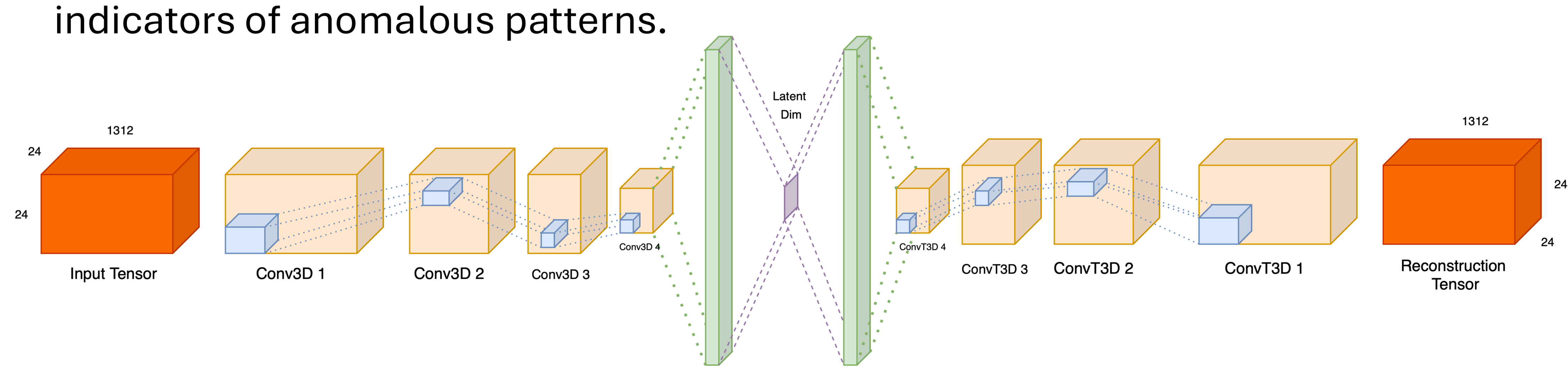
- Spectra act as chemical fingerprints, allowing for the characterization of nanoscale materials.
- Manual analysis is currently required for subtle spectral anomaly detection.
- Principal Component Analysis (PCA) struggles with complex features and reliable anomaly detection.

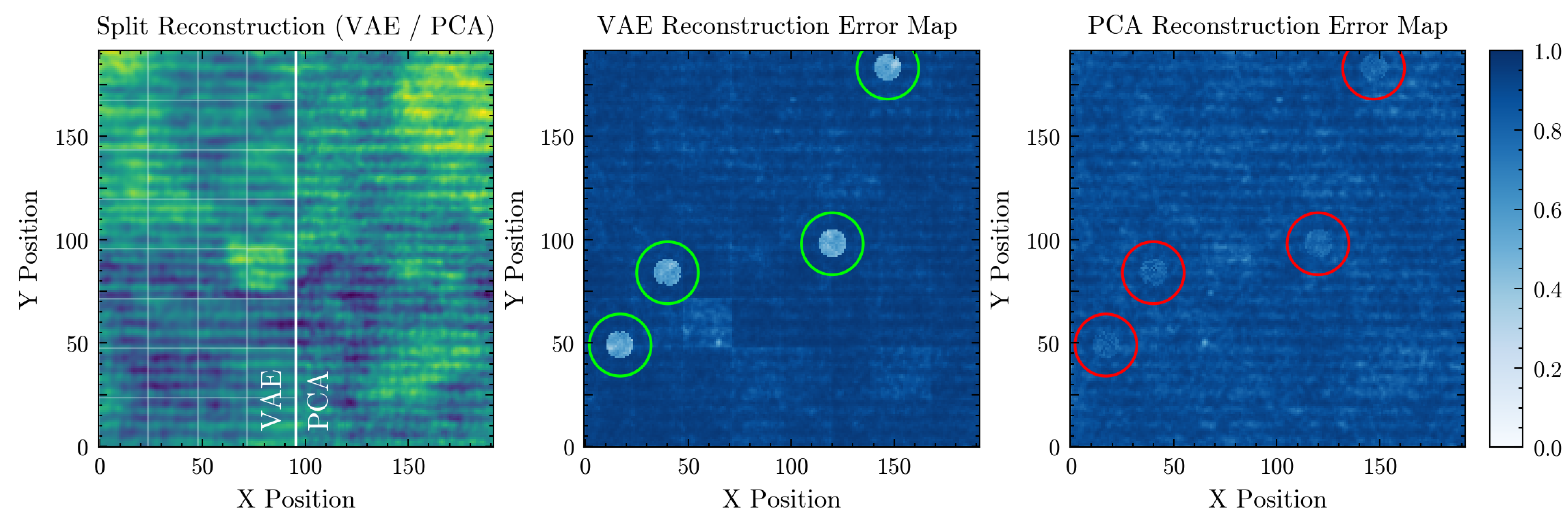
Methods

- Develop 3D Convolutional Variational Autoencoder (3D-CVAE) for EELS-SI analysis.
- Use negative log-likelihood loss to handle discrete energy channels.
- Processes full 3D data cube while preserving spatial relationships.
- Autoencoder's bottleneck architecture forces learning of essential normal features, making reconstruction errors effective indicators of anomalous patterns.



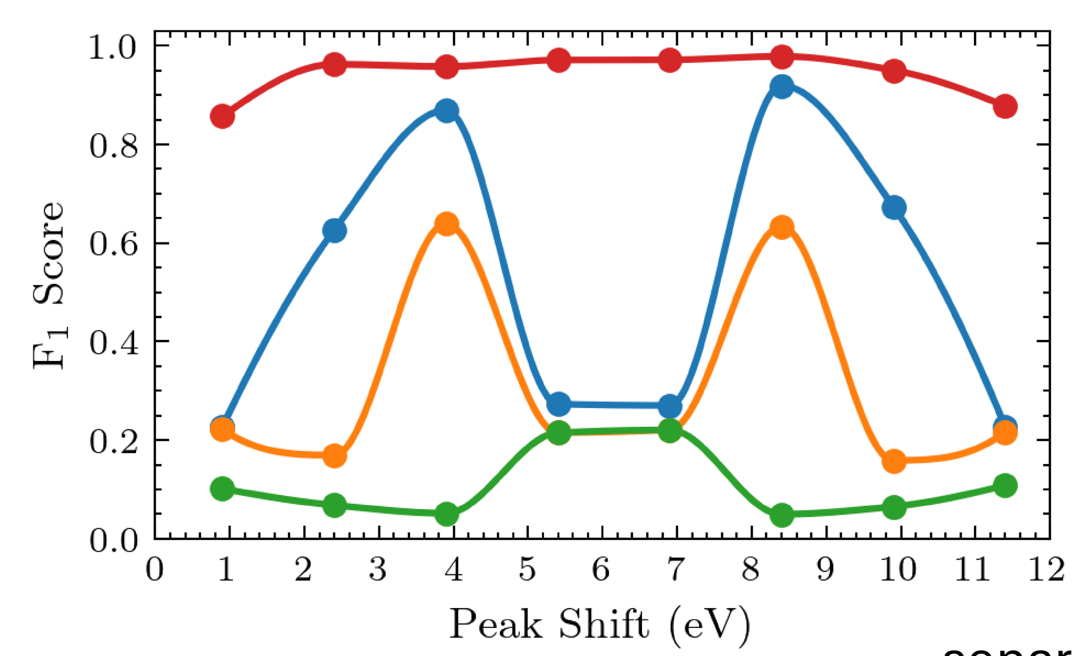
- Train model on normal (black) spectra to learn normal features.
- Validate approach using iron spectrum (L edge) artificial peak shift anomalies (red).





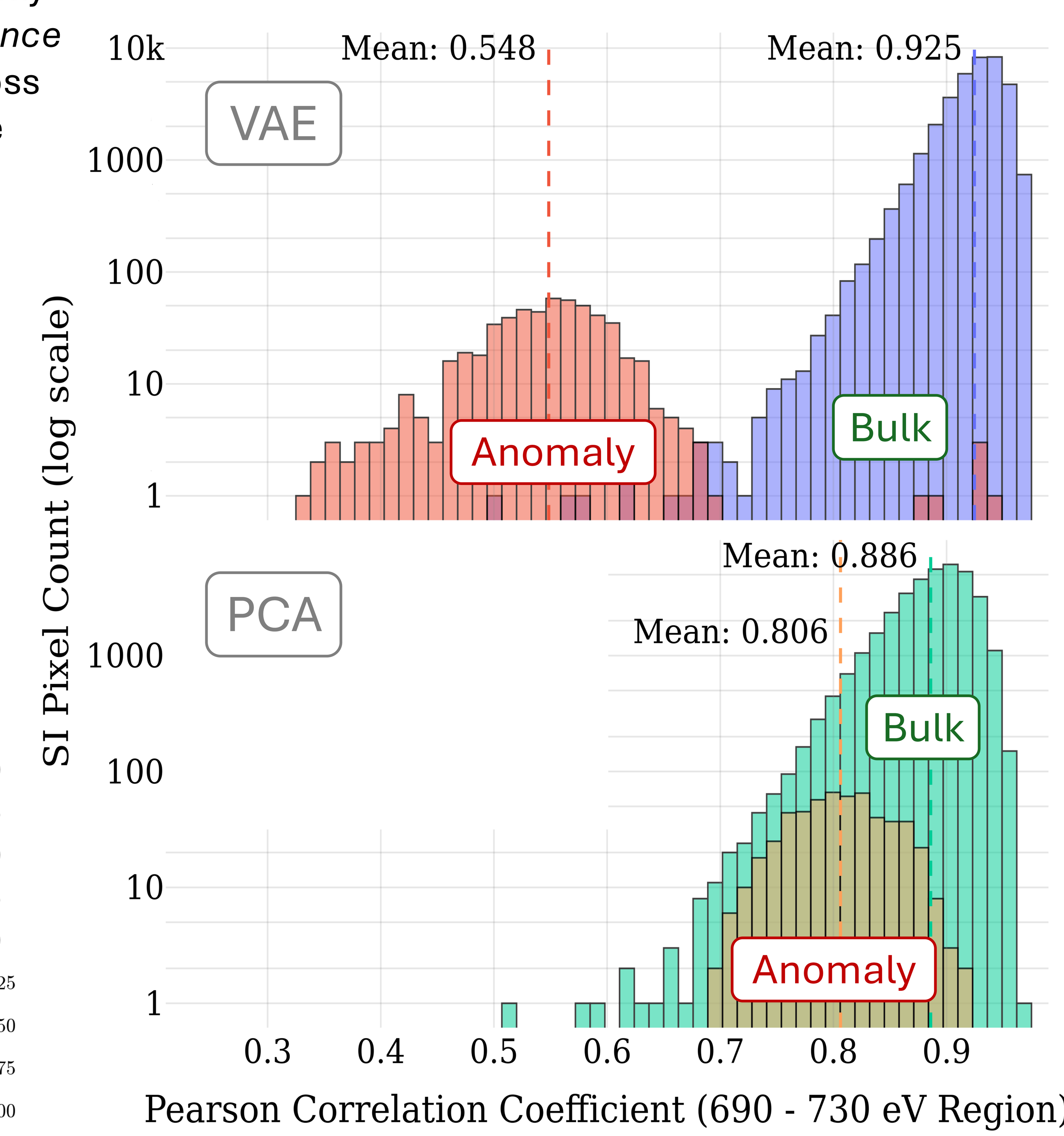
Results

A two-dimensional representation of the data cube containing both normal spectra and anomalies. The data cube was reconstructed using both VAE and PCA. Analysis of the data cube shows that anomalies are clearly identified using VAE (green circles), while PCA does not separate them (red circles) significantly from the rest of the spectral data.

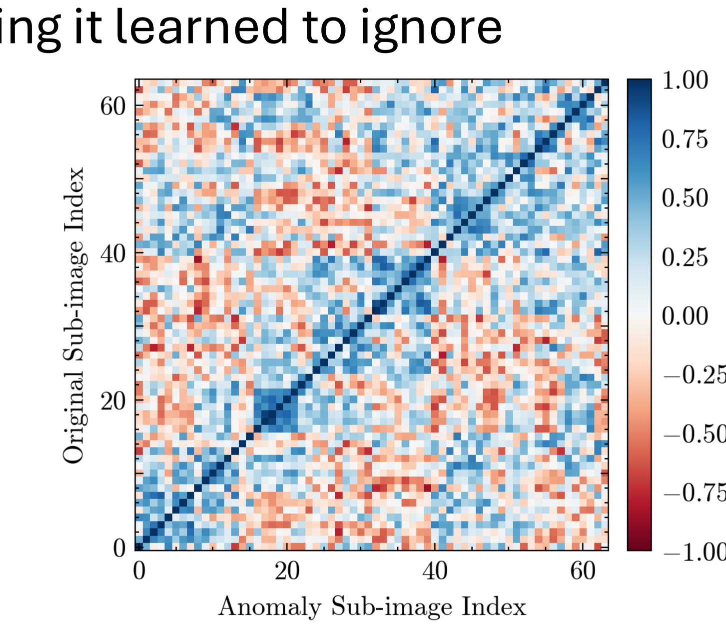


Our approach (VAE) maintains consistently high detection accuracy *(F1-scores balance true positives with false detections)* across various shift magnitudes *(red line)*, while PCA's performance varies significantly *(blue, orange, green for PCA with 3, 4, 5 components respectively)*

VAE outperforms PCA in anomaly detection, shown by clear bimodal separation in Pearson Correlation Coefficient distributions with only six misclassifications out of 38,000 pixels



When our model processes both normal and anomaly-containing data, it recognizes them as essentially the same (Blue diagonal), showing it learned to ignore defects and maintain the underlying normal pattern: exactly what we want for anomaly detection.



Conclusion

- 3D-CVAE demonstrates superior EELS-SI anomaly detection over PCA, with consistent performance across shift magnitudes
- Our method maintains reconstruction fidelity in noise-dominated regions despite diminishing advantage over PCA at low anomaly concentrations

Acknowledgments

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