Data-driven model for fingerprinting plastic waste material using low-cost spectroscopy

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Who am I?

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Agenda

- Three works:
  - The enabling technologies for digitalization in the chemical process industry **(published)**
  - Capturing variability in material property predictions for plastics recycling via machine learning **(published)**
  - Data-driven model for fingerprinting plastic waste material using low-cost spectroscopy **(in progress)**

The enabling technologies for digitalization in the chemical process industry

Motiation

- **Chemical process industry lags** behind other sectors in digitalization
- Barriers: **high costs**, **lack of digital culture/training**, **unclear vision**
- **Objective:** Provide a **structured overview** of enabling technologies for practitioners with little/no digitalization background
- Goals:
  - Identify and categorize enabling technologies
  - Link industry **problem domains** with digital **development aspects**
  - Showcase **case studies** of underutilized but high-potential technologies

Problem Domains

Maintenance

Production

Safety

Supply Chain

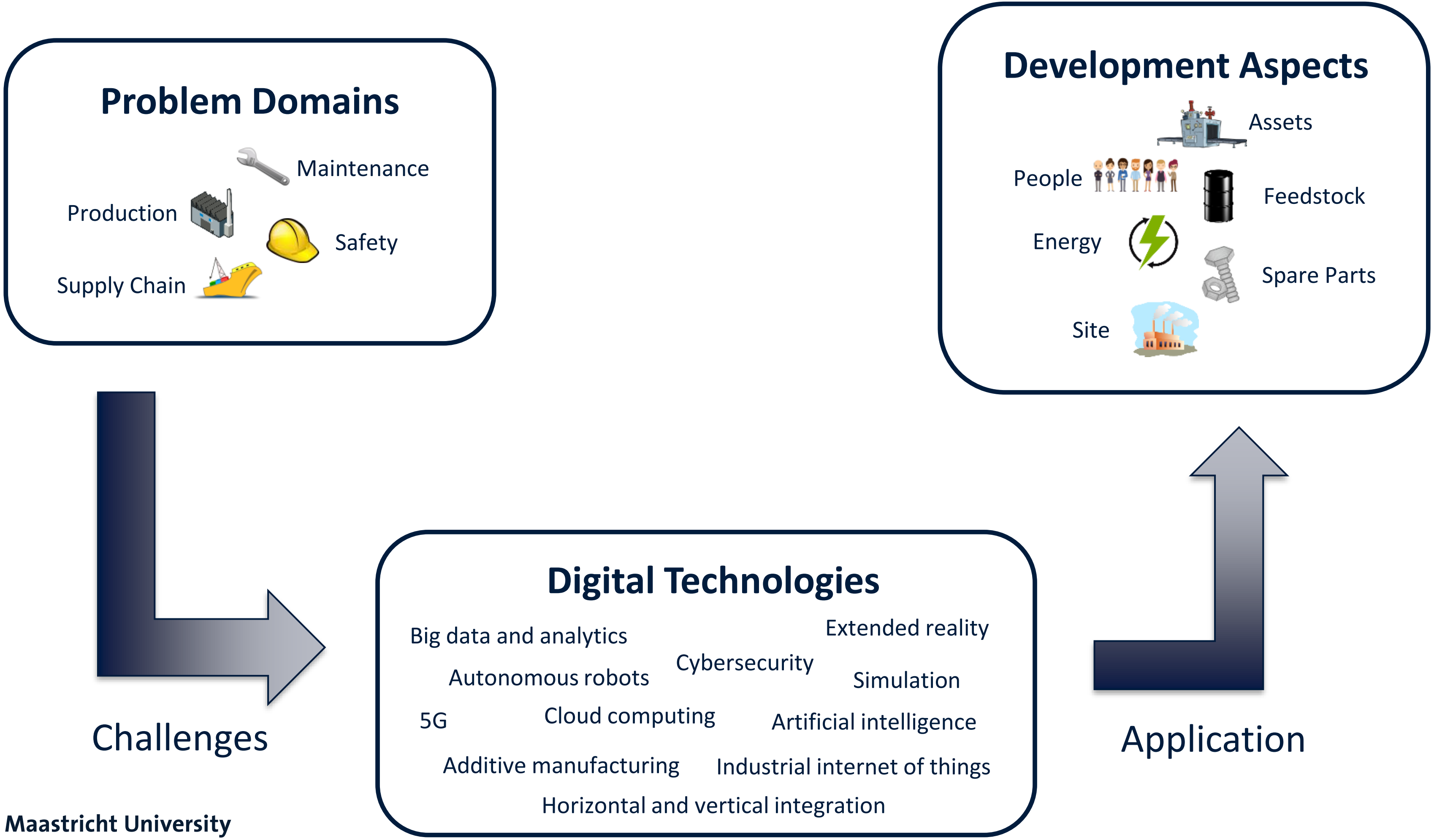
Problem Domains

- Maintenance
- Production
- Safety
- Supply Chain

Challenges

Digital Technologies

- Big data and analytics
- Extended reality
- Cybersecurity
- Autonomous robots
- Simulation
- 5G
- Cloud computing
- Artificial intelligence
- Additive manufacturing
- Industrial internet of things
- Horizontal and vertical integration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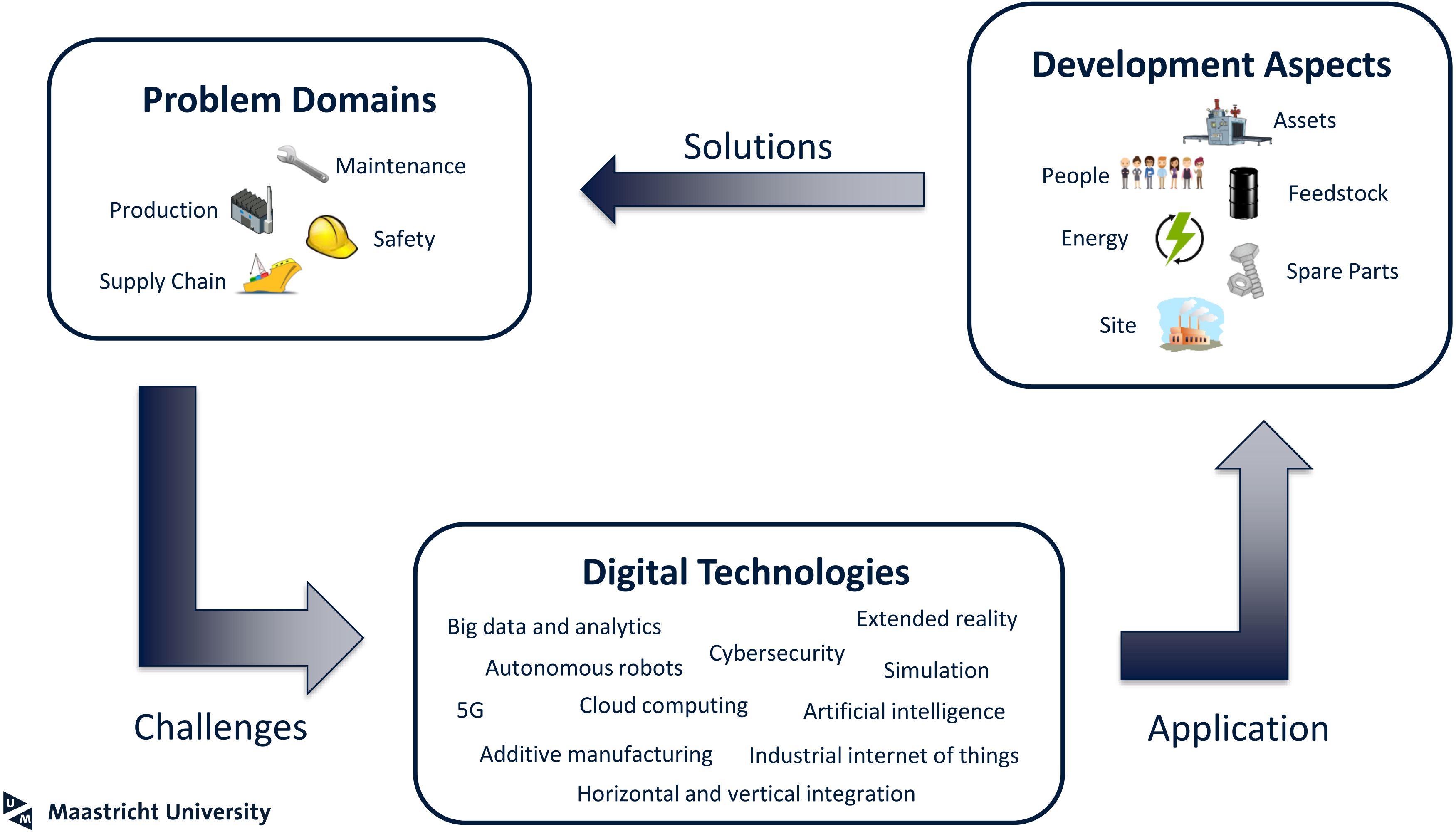
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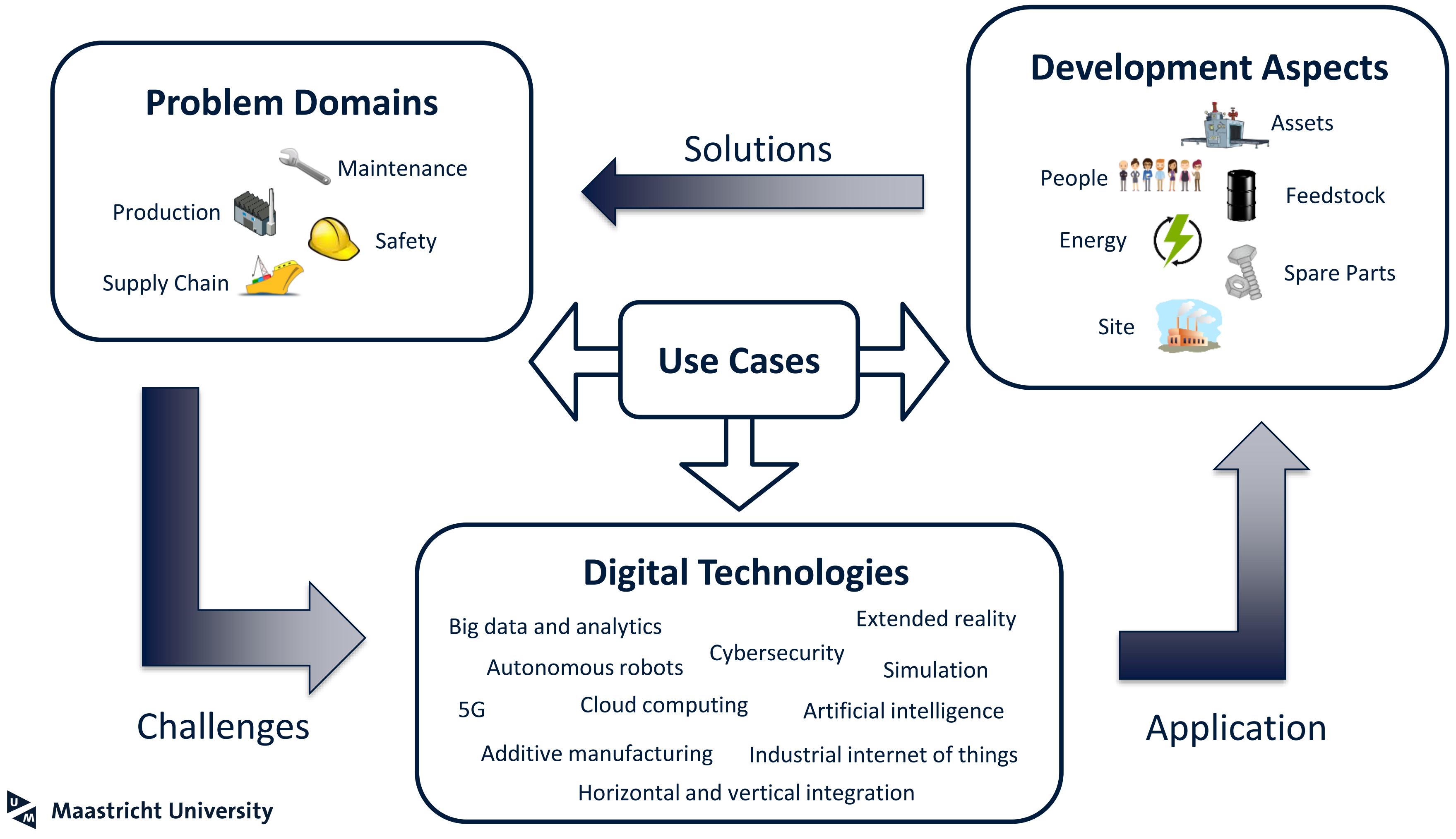

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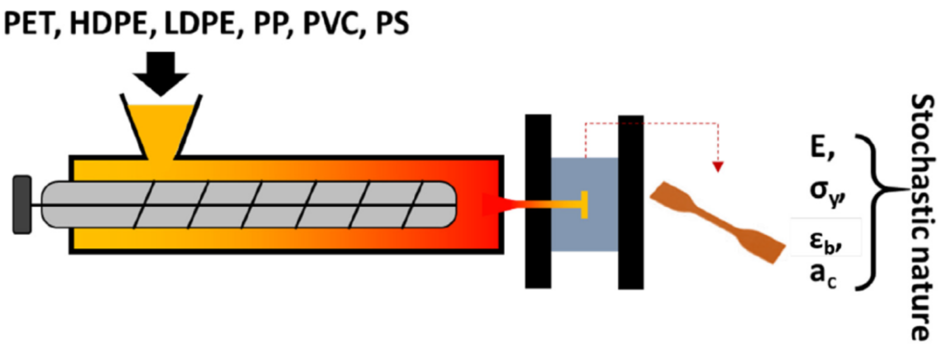
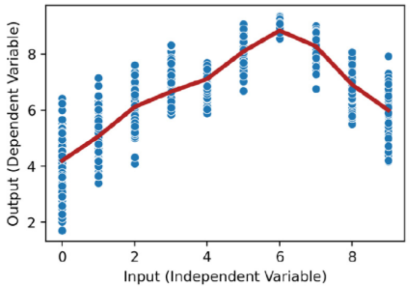
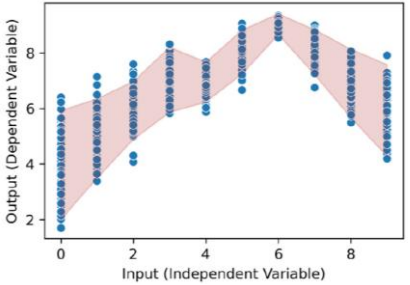
Capturing variability in material property predictions for plastics recycling via machine learning

Motivation

- Blends of waste plastics → **nonlinear and stochastic properties**
- Traditional ML models predict **single values** (point estimates) → insufficient to capture uncertainty
- **Key research gap:** Need methods that predict **ranges of properties** (intervals) to account for variability

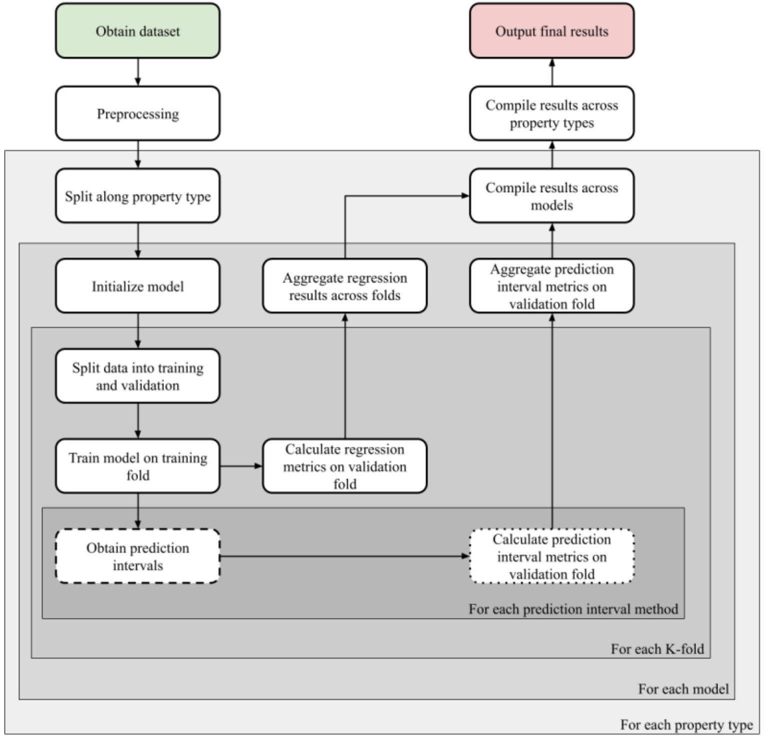






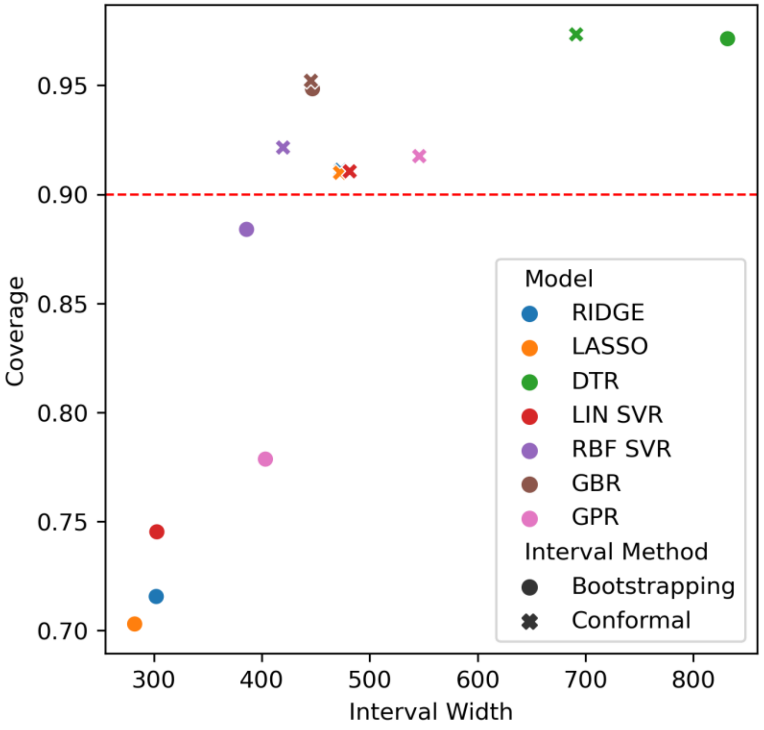
Methodology

- Dataset: **3352 samples**, 10 virgin polymers, tested in blends
- Target properties: Elastic modulus (E), Yield strength (σy), Strain at break (εb), Impact strength (ac)
- Models tested: **Ridge, Lasso, SVR, Decision Trees, Gradient Boosting, Gaussian Process**
- Interval methods: **Residuals, Bootstrapping, Conformal Predictions**
- Evaluation: RMSE, Coverage, Interval Width



Results

- **Gradient Boosting and SVR** best for **point predictions**
- **Conformal predictions** best for **interval accuracy**
- Demonstrates the use of interval-based machine learning to capture the variability in the mechanical properties of heterogeneous plastic blends



Data-driven model for fingerprinting plastic waste material using low-cost spectroscopy

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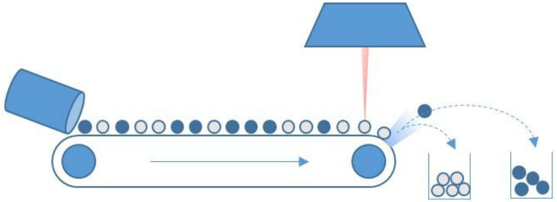
The Plastic Waste Problem

- Plastics are ubiquitous: durable, lightweight, cheap
- But…
  - 12 billion tonnes projected in landfills and ecosystems by 2050
  - Only 9 percent of plastics globally are recycled with over 70 percent ending up in sanitary landfills and uncontrolled dumpsites (OECD)
  - Mismanaged plastic is a major contributor to the environmental crisis
- Mechanical recycling = scalable circular economy approach
- **Challenge:** plastics are chemically diverse and thus need **accurate separation**
  - Poor sorting → contamination → degraded material quality → reduced economic viability

Spectroscopy in recycling

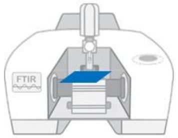
- Vibrational spectroscopy → unique **spectral fingerprints** of polymers
- Advantages: fast, non-destructive, automated
- Near-Infrared (NIR, 1000–2500 nm) widely used with ML
- State of the art → high-cost, wide-band spectrometers
- **Gap:** limited research on low-cost, narrow-band devices (<1100 nm)



Conveyor Spectral Sorting

Pros
- Very fast scanning speed
- Direct sorting of materials

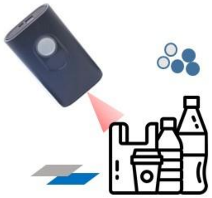
Cons
- Large monetary investments
- Practically immovable



Benchtop Spectroscopy

Pros
- High spectral quality
- Transportable device

Cons
- Inflexible operation
- Sample preparation often needed



Handheld Spectroscopy

Pros
- Low-cost implementation
- Highly portable for many applications

Cons
- Slight lower data quality

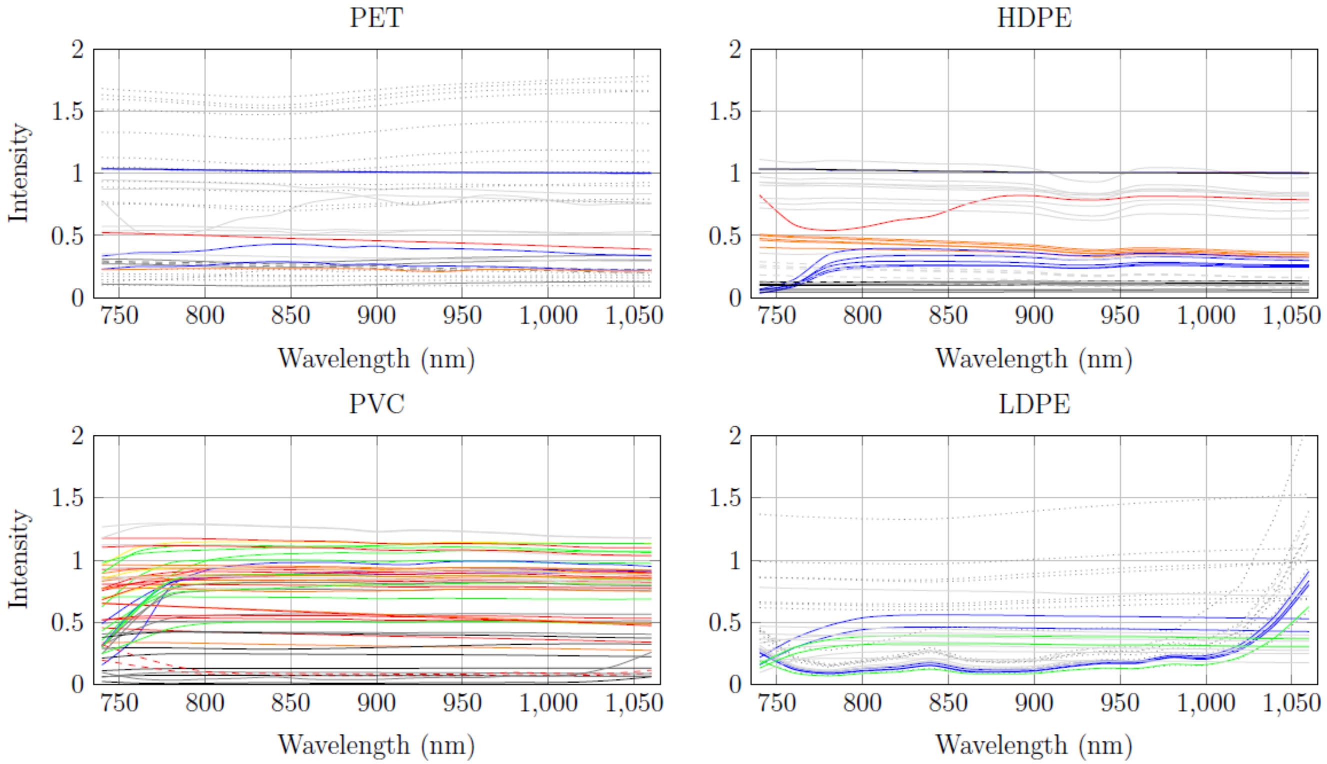
Objectives

- Assess feasibility of low-cost, narrow-band NIR spectroscopy (740–1070 nm) for classifying plastics.
  - Make classification accessible in **resource-limited environments**
  - Potential to enable recycling **at point of collection** → less contamination downstream
- **Research question:** *Can consumer-grade, narrow-band NIR spectroscopy + ML accurately classify plastic waste?*
- **Tasks:**
  - Collect **novel dataset** of household plastics (7 types).
  - Develop **machine learning** pipeline for classification.
  - Benchmark against existing approaches.

Data collection

- Data collection performed by students on-site at Chemelot
- Househouse plastic waste
- Device: **SCiO Mini spectrometer** (740–1070 nm)
- Samples: **363 data points** (7 classes: PET, HDPE, PVC, LDPE, PP, PS, Other)
- Features:
  - **Spectral** (wavelength intensities)
  - **Categorical** (color, transparency)

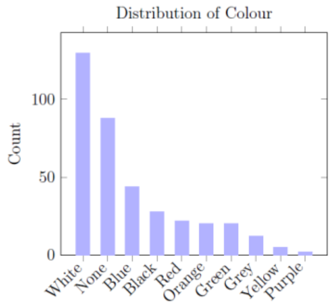
Data collection

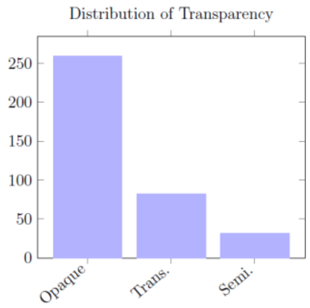


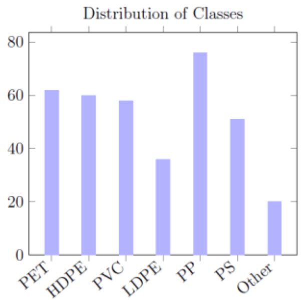
Data insights

- Imbalance observed:
  - Color → white/transparent/opaque overrepresented
  - Class sizes uneven

	White	None	Blue	Black	Red	Orange	Green	Grey	Yellow	Purple	Opaque	Trans.	Semi.
PET	15	36	4	0	1	1	0	5	0	0	26	33	3
HDPE	25	0	17	8	1	9	0	0	0	0	55	0	5
PVC	9	0	3	6	14	7	9	7	3	0	56	0	2
LDPE	14	14	5	0	0	0	3	0	0	0	21	14	1
PP	28	12	13	5	3	2	7	0	4	2	61	10	5
PS	17	23	1	9	0	1	0	0	0	0	28	23	0
Other	19	1	0	0	0	0	0	0	0	0	7	0	13

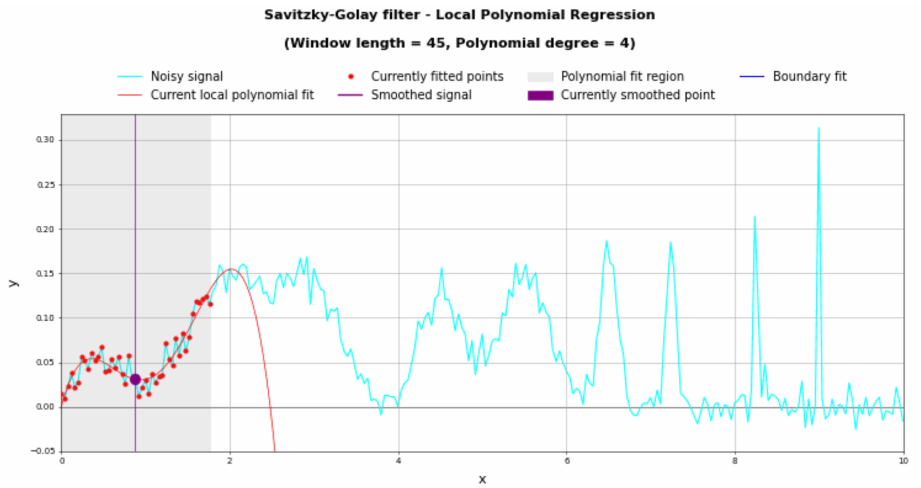


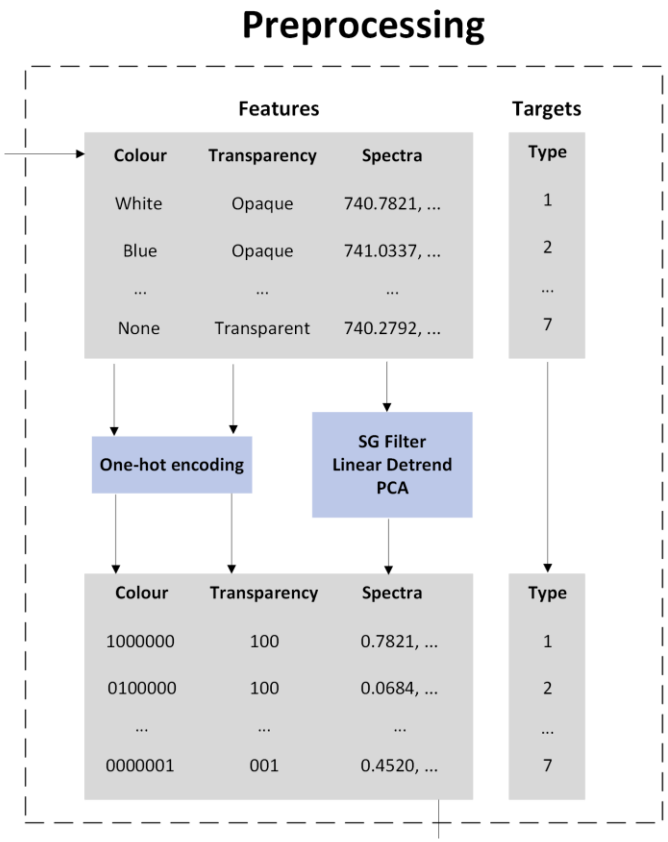




Data preprocessing

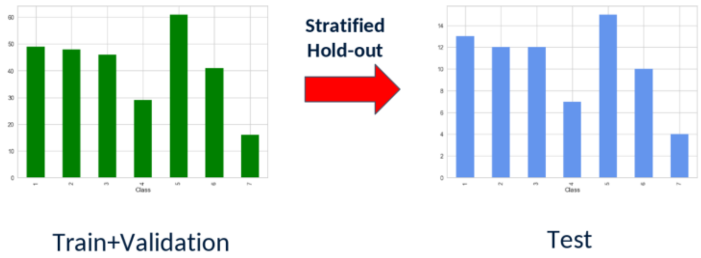
- Categorical features:
  - **One-hot encoding**
- Spectra:
  - **Savitzky-Golay filter** → smooth and enhance spectral features
  - **Linear detrending** → remove baseline shifts
  - **PCA** → dimensionality reduction (model-dependent benefits)

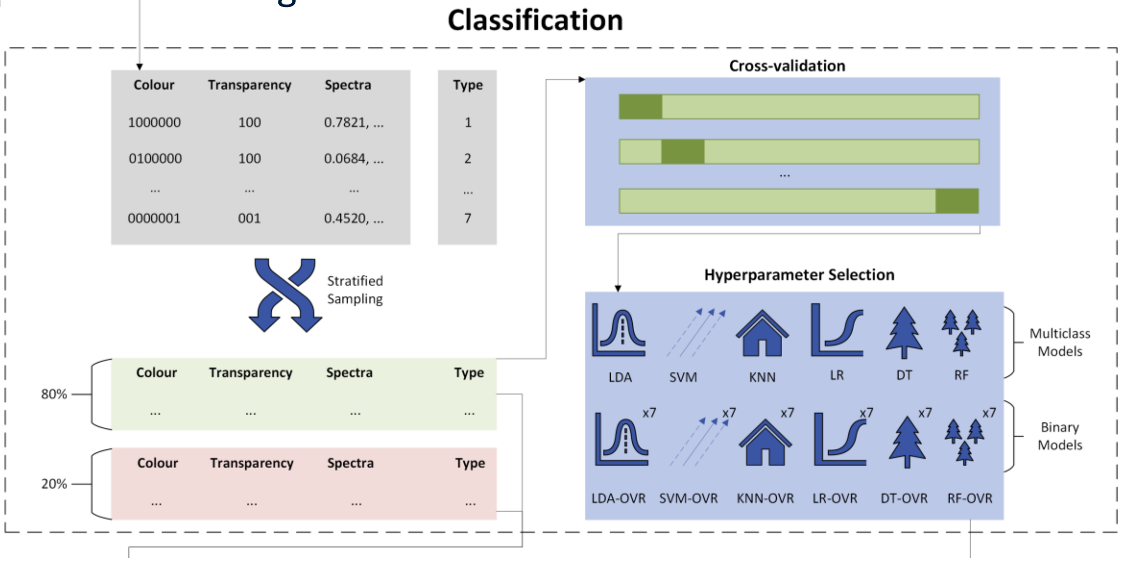




Classification paradigms

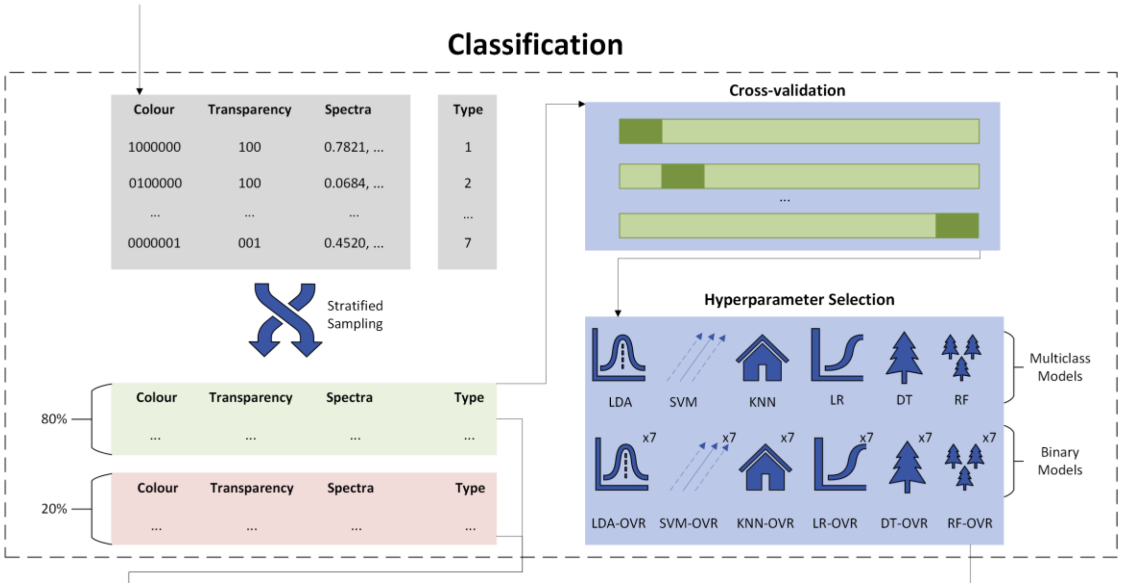
- **Multiclass Classification**: predict 1 of 7 classes directly
- **One-vs-Rest (OVR)**: 7 binary classifiers, combined
- Tradeoff:
  - Multiclass = simpler, faster
  - OVR = sometimes better accuracy and robustness
- **10-fold Cross-Validation** for hyperparameter tuning





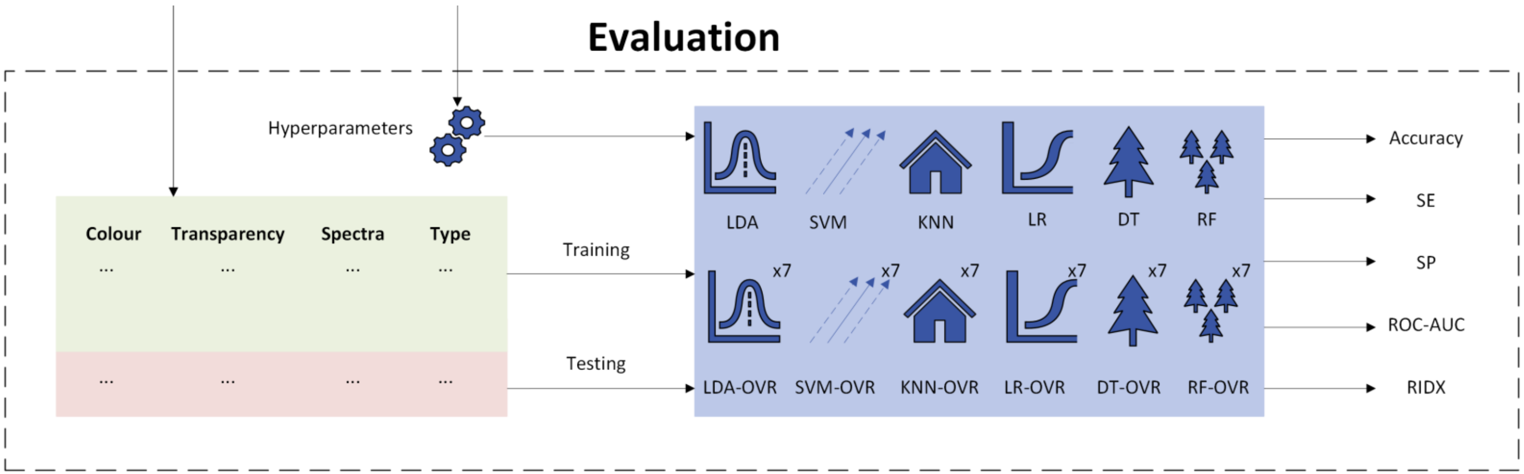
Classification models

- Linear Discriminant Analysis (LDA)
- Support Vector Machines
- K-Nearest Neighbours (KNN)
- Logistic Regression (LR)
- Decision Trees (DT)
- Random Forest (RF)



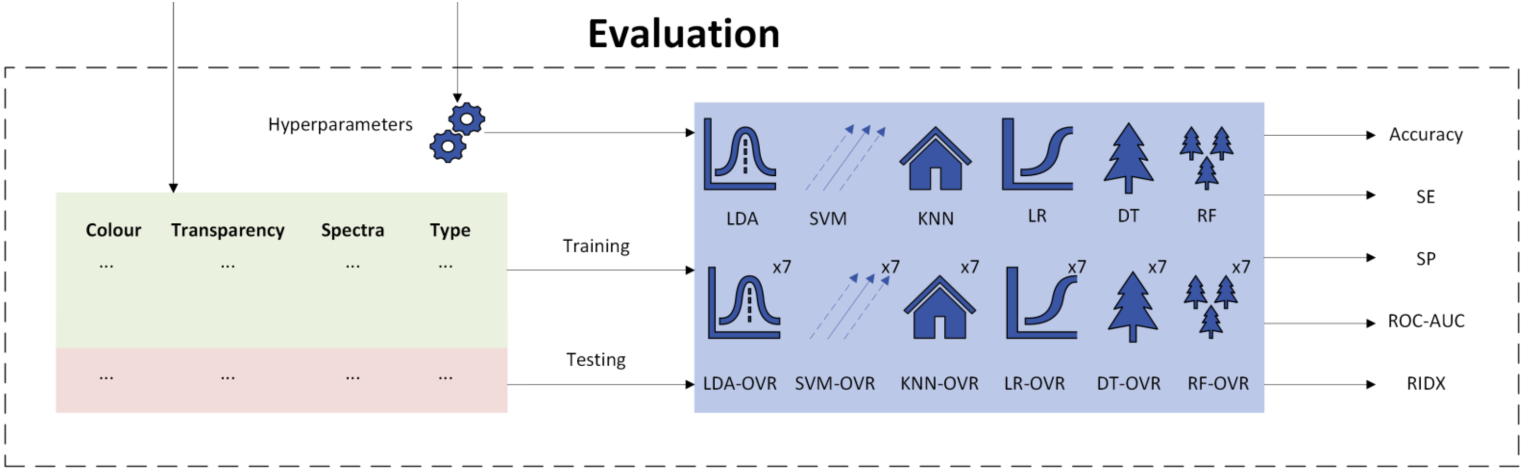
Evaluation setup

- **Holdout test set** (20%) for final evaluation.
- Stratified sampling to preserve class proportions.
- Metrics: Accuracy, Sensitivity, Specificity, ROC-AUC, **RIDX**.



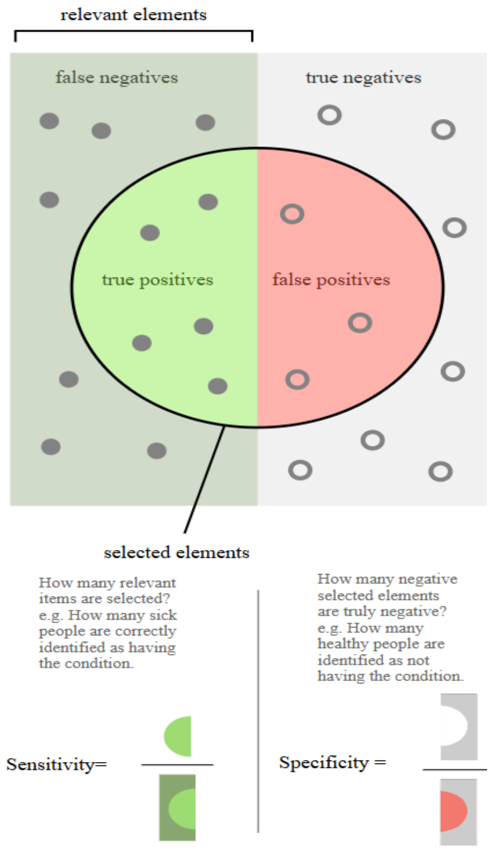
Why evaluation metrics matter?

- Accuracy **NOT** enough: doesn't capture *what* was misclassified
- In recycling, **cost of errors** differs:
  - Misclassifying PVC as PET is much worse than misclassifying PET as HDPE
- Need metrics that reflect **real-world recycling impact**



Standard metrics used

- **Accuracy** – proportion of correct predictions
- **Sensitivity (Recall)** – correctly identified positives
- **Specificity** – correctly identified negatives
- **ROC-AUC** – ability to separate classes across thresholds



Recyclability Index (RIDX)

- Novel metric proposed in this work
- Captures **cost of misclassification** based on recycling compatibility

$$\mathrm{RIDX} = 1 - \frac{\sum F_{ij} \times w_{ij}}{\sum F_{ij} \times \max(w_{ij})}$$

- Values between **0 (worst)** and **1 (perfect classification)**
- Rule: **Misclassifying harder-to-recycle plastics as easier ones = higher penalty**

		Predicted						
		PET	HDPE	PVC	LDPE	PP	PS	Other
Actual	PET	0	1	2	2	2	2	2
	HDPE	1	0	2	2	2	2	2
	PVC	6	6	0	6	6	5	5
	LDPE	4	4	4	0	3	4	4
	PP	4	4	4	3	0	4	4
	PS	6	6	5	6	6	0	5
	Other	6	6	5	6	6	5	0

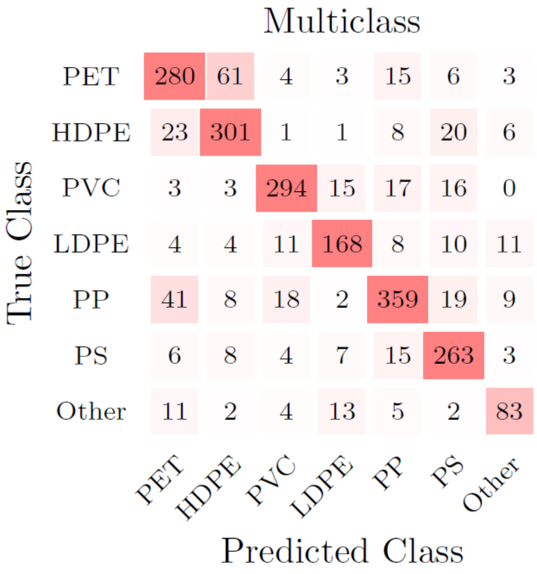
Results

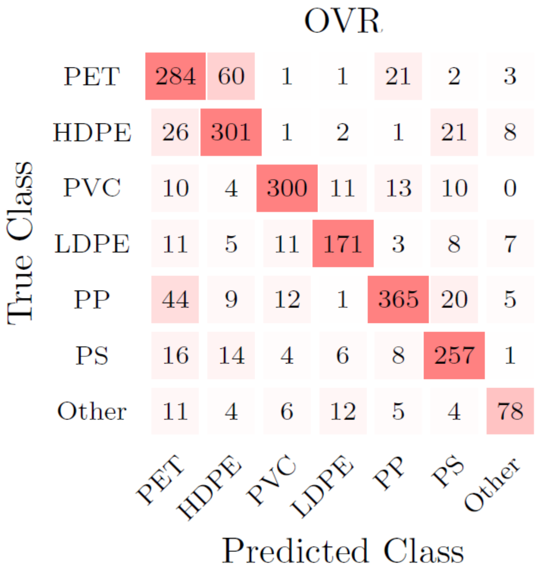
- Best performer: **SVM (One-vs-Rest)**
- Accuracy: **87%**
- Both multiclass and OVR similar structure, OVR slightly better

Model	Accuracy	SE	SP	ROC-AUC	RIDX
LDA	0.7904	0.7782	0.9650	0.9379	0.8726
LDA - OVR	0.7763	0.7574	0.9624	0.9365	0.8568
SVM	0.8404	0.8459	0.9731	0.9822	0.9124
SVM - OVR	**0.8676**	**0.8656**	**0.9778**	0.9730	**0.9297**
KNN	0.8016	0.7916	0.9662	0.9578	0.8713
KNN - OVR	0.8096	0.7968	0.9677	0.9600	0.8776
LR	0.8347	0.8401	0.9721	0.9687	0.9095
LR - OVR	0.8512	0.8412	0.9747	0.9702	0.9150
DT	0.6884	0.6579	0.9470	0.8397	0.7960
DT - OVR	0.6910	0.6675	0.9470	0.9267	0.7972
RF	0.8593	0.8464	0.9761	0.9751	0.9200
RF - OVR	0.8399	0.8247	0.9732	**0.9770**	0.9075

Results

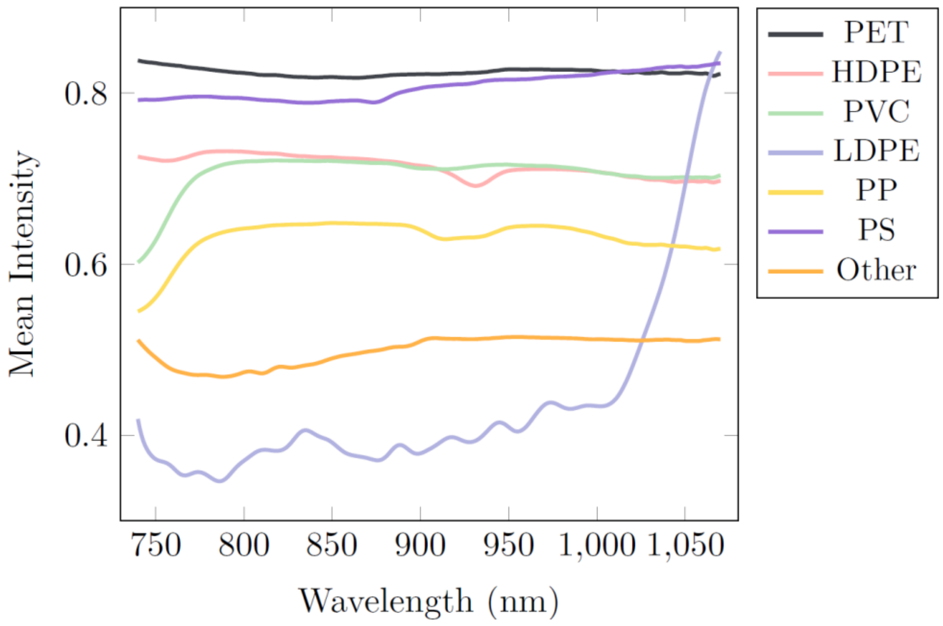
- Misclassifications observed:
  - PET ↔ HDPE (most common)
  - PP misclassified as PET





Results

- Mean aggregated spectra → good separability, but **sample-level variance matters**



Results

- Tested dropping key pipeline components:
  - **Categorical features (color, opacity):** performance drops sharply
  - **Preprocessing (SG filter + detrending):** essential for SVM, KNN
  - **PCA:** mixed results → helps some models, hurts others
- Conclusion: **categorical features and preprocessing are critical**
- Future direction: **multi-sensor fusion** (cheap colorimeters + spectrometers)

	Ablation					
Model	None	CAT	PR	PCA	CAT&PCA	PR&PCA
LDA	0.7904	0.7410	0.7874	**0.7959**	0.7495	0.7548
LDA - OVR	**0.7763**	0.7381	0.7819	0.7683	0.7244	0.7352
SVM	0.8404	0.7964	0.5675	**0.8586**	0.7906	0.5620
SVM - OVR	**0.8676**	0.7769	0.5809	0.8511	0.7709	0.5698
KNN	0.8016	0.7602	0.6026	**0.8155**	0.7736	0.6026
KNN - OVR	**0.8096**	0.7518	0.6054	0.7931	0.7576	0.6026
LR	0.8347	0.7576	0.7656	**0.8514**	0.7658	0.7655
LR - OVR	0.8512	0.7654	0.7488	**0.8594**	0.7629	0.7543
DT	0.6884	0.6060	0.7076	**0.7577**	0.7353	0.4732
DT - OVR	**0.6910**	0.6247	0.6498	0.6806	0.6783	0.5261
RF	0.8593	0.8398	0.8538	**0.8597**	0.8322	0.5262
RF - OVR	0.8399	0.8263	0.8593	**0.8677**	0.8372	0.5017

Comparison with prior work

- Wide-band devices (>1200 nm) → accuracies **>95%** (CNN, SVM, etc.)
- Despite limits → achieved **best reported performance below 1100 nm**

Citation	Device	Type	Band (nm)	Model	# Samples	# Classes	Accuracy
2020 [75]	Pynect NIR-S-G1	Handheld	900 - 1700	SVM	1800	7	1.000
2021 [35]	NIRQuest 512-1.7	Benchtop	900 - 1700	CNN	512	5	0.984
2021 [34]	NIR512	Benchtop	900 - 1700	Combined	200	7	0.957
2021 [76]	ASD FieldSpec 4	Handheld	350 – 2500	PLS-DA	36	2	0.806
2021 [36]	MicroNIR Pro ES 1700	Handheld	950 - 1650	CNN	759	7	0.980
2022 [37]	NIR17S	Benchtop	900 - 1700	CNN	650	3	0.978
2023 [38]	Helios-G2–320	Conveyor	930 - 1700	CNN	31500	7	0.999
2023 [44]	IAS-5000	Handheld	900 - 1700	SVM	60	4	0.980
2023 [41]	Resonon Pika NIR-320	Conveyor	900–1700	ANN	1080	4	0.895
2023 [58]	MicroNIR Pro OnSite	Handheld	950 - 1650	Combined	1625	4	0.990
2023 [49]	Custom	Handheld	750 - 1050	CNN	64	5	0.621
2024 [39]	AS7265X	Handheld	410 - 940	CNN	1200	6	0.725
2024 [77]	IS10	Benchtop	900 - 1700	PLS-DA	298	5	0.975
2025 [42]	IS10	Benchtop	900 - 1700	GAN	250	5	0.980
2025 [48]	Bruker Vector 22/N NIR	Benchtop	800 - 1700	KNN	142	5	1.000
2025 [28]	Avaspec-NIR256-2.0TEC	Benchtop	1000 - 2000	RF	813	7	0.974
Our work	SCiO Mini	Handheld	740 - 1070	SVM - OVR	363	7	0.867

Summary and future work

- **ML + NIR is feasible:** even low-cost consumer devices can classify plastics
  - Data fusion of categorical features improves results

- Only **household plastics** included → may not generalize to industrial waste
- **Small dataset (363 samples):** limits use of deep learning
  - **Expand dataset** → more samples, more diverse plastics
  - **Deep learning** (CNN, GANs) when data volume allows
- **Multi-sensor fusion:** combine cheap sensors (colorimeter, opacity)

- **Next step:** finish paper for Waste Management Journal

Thank you

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