

# Raman Mineral Classification

A Multi-Approach Machine Learning Analysis

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# Introduction

## Context

Raman spectroscopy enables detailed chemical analysis of minerals through spectral signature interpretation.

## The Problem

Manual classification of spectral signatures is time-consuming and error-prone.

## The Goal

Automate classification of 7 minerals: Albit, Calcite, Dolomit, Feldspat, Quarz, Rhodocrosite, Tile.

# Project Objectives

- **Develop a Hybrid System:** Compare Supervised, Unsupervised, and Classical approaches
- **High Accuracy:** Target >95% accuracy across all classes
- **Scalability:** Efficiently handle large datasets (1 FPS and 30 FPS)
- **Robustness:** Ensure consistent performance regardless of sampling rate

# Methodology Overview

## Three Distinct Approaches

### Supervised

ResNet-18 CNN for direct image classification

### Unsupervised

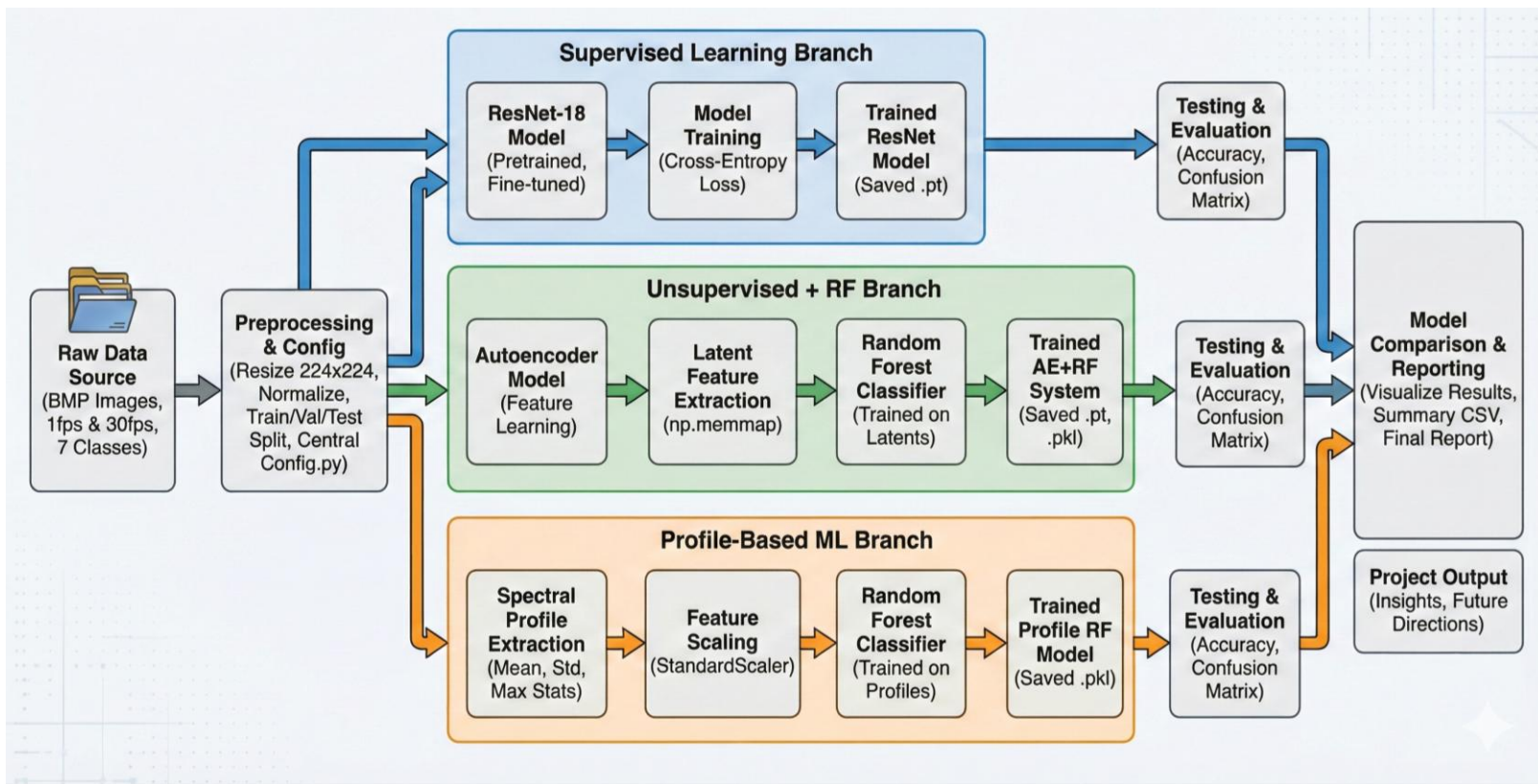
Autoencoder + Random Forest for feature learning

### Classical

Profile Statistics + Random Forest with handcrafted features

**Global Settings:** Images resized to 224×224 | SEED=42 | GPU: CUDA

# Workflow Overview



# Method 1: Supervised Learning (ResNet-18)

## Architecture

ResNet-18 pretrained on ImageNet with final layer adapted for 7 classes

## Training Configuration

Cross-Entropy Loss | Fine-tuned for 5 epochs | Rapid convergence

## Key Advantage

Fast convergence and high accuracy with minimal computational overhead

# Method 2: Unsupervised (Autoencoder + RF)

## Step 1: Autoencoder

Compresses images to latent vectors (dim=64) | MSE Loss minimization

## Step 2: Feature Extraction

Latent features saved to disk using Memory Mapping for efficiency

## Step 3: Classification

Random Forest trained on extracted latent features

**Concept:** Learn features without labels first, then classify

# Method 3: Classical ML (Profile Statistics)

## Data Source

Raw spectral profiles from CSV files

## Feature Engineering

Statistical moments extracted: Mean, Standard Deviation, Max, Min

## Pipeline

Standardization (StandardScaler) → Random Forest (300 estimators)

## Advantages

Extremely fast, highly interpretable, CPU-friendly, no GPU required

# Key Challenges & Solutions

## Dataset Idealism vs. Real-World Noise:

- 100% accuracy suggests pure lab samples.
- Model may struggle with "dirty" field data (fluorescence, low signal-to-noise).

## Restricted Class Scope:

- Limited to 7 specific minerals (no "Unknown" category).
- Risk of false positives if an unlisted mineral is analyzed.

## Lack of Mixed-Phase Detection:

Assumes single mineral per image.

Cannot quantify mixtures or those outside scope of training (e.g., rocks containing both Quartz and Feldspar).

# Results Summary

## Performance

**100% Accuracy** achieved on test sets across all three methods

## Consistency

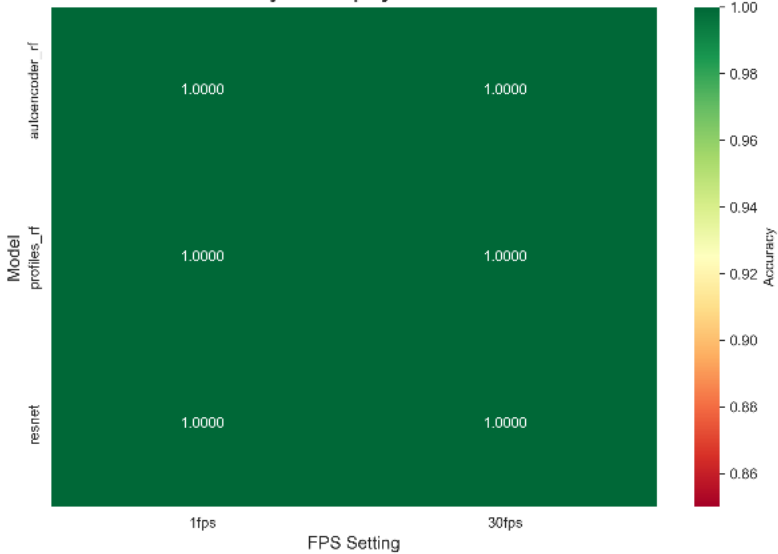
Identical results for both 1 FPS and 30 FPS datasets

## Inference Comparison

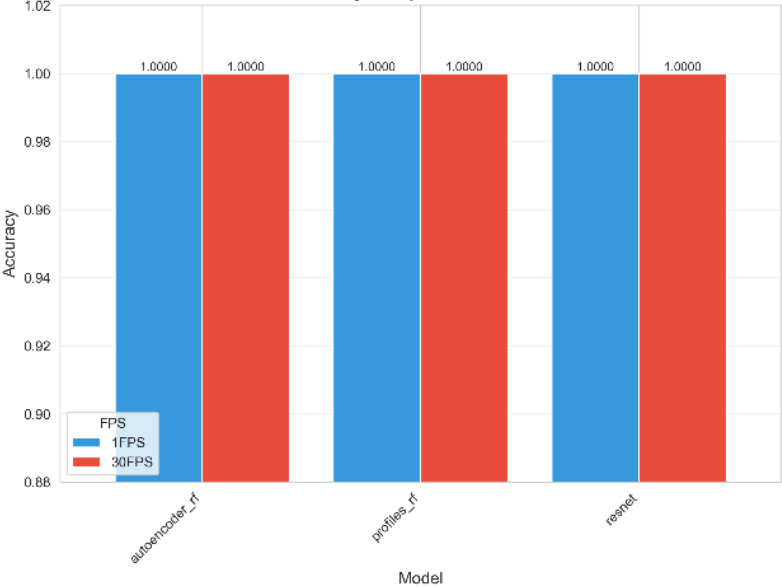
- **ResNet:** Fast, GPU-dependent training
- **Profiles RF:** Fastest, CPU-friendly

# Results Visualizations

Accuracy Heatmap by Model & FPS



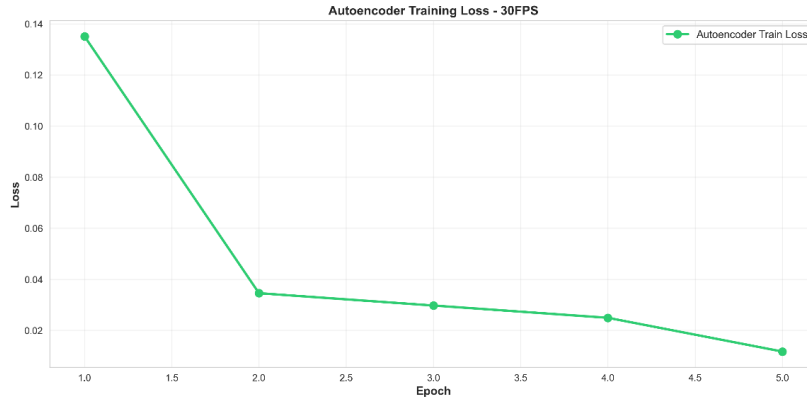
Model Accuracy Comparison: 1FPS vs 30FPS



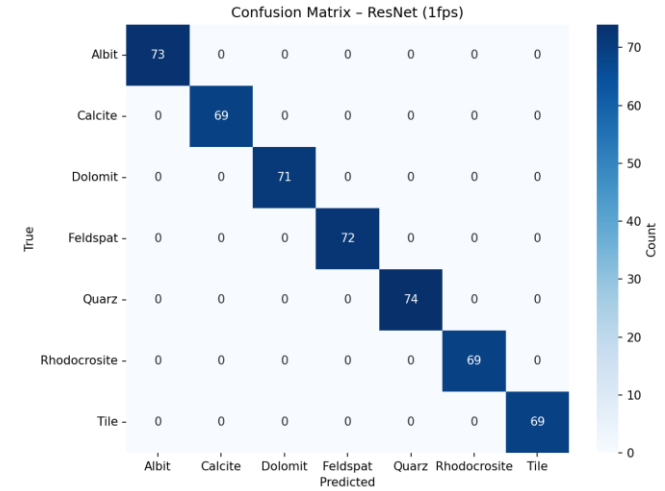
**Confusion Matrices:** Zero misclassifications across all 7 classes

**Bar charts:** Charts showing 100% accuracy across all models

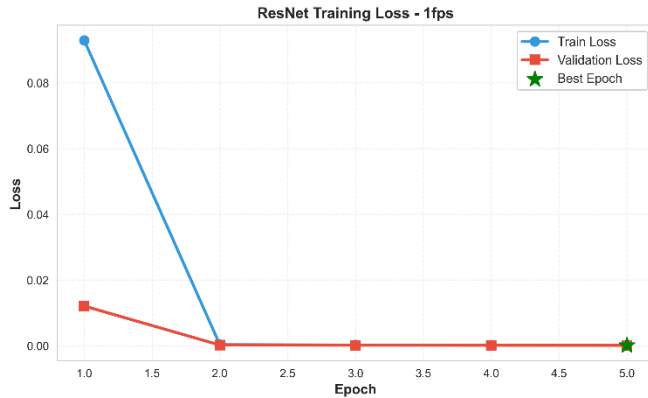
(Cont.)



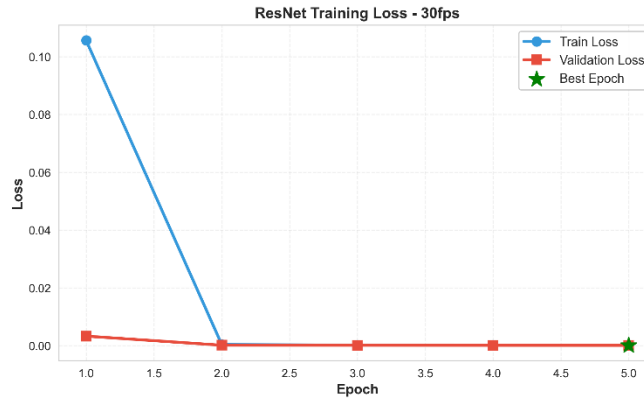
Autoencoder Training Loss Curve(30 FPS)



ResNet Confusion Matrix 1 FPS



ResNet Training Loss Curve



# Results: Tables

Table 1: ResNet-18 Training History (1 FPS)

Epoch	Train Loss	Val Loss	Val Acc
1	0.0929	0.0121	100%
2	0.0003	0.0002	100%
5	0.0001	<0.0001	100%

Table 2: Autoencoder Training History (30 FPS)

Epoch	Train Loss	Val Loss
1	0.1351	0.0357
3	0.0297	0.0273
5	0.0117	0.0023

Table 3: Profile RF Performance

Dataset	Samples (Train)	Samples (Test)	Estimators	Accuracy
1 FPS	122,810	13,646	300	100%
30 FPS	134,986	14,999	300	100%

Table 4: Accuracy metrics across all three implemented architectures

Experiment	FPS	Accuracy	Test Samples
resnet	1fps	1	497
resnet	30fps	1	506
autoencoder_rf	1fps	1	497
autoencoder_rf	30fps	1	506
profiles_rf	1fps	1	13646
profiles_rf	30fps	1	14999

# Conclusion & Acknowledgments

## Key Finding

Raman spectral data for these minerals is highly distinct. Both Deep Learning and Classical methods are viable.

## Limitations

High accuracy suggests ideal lab data | Limited to 7 known classes | May struggle with mixed samples

190.015 Applied Machine and Deep Learning WS25/26, Montanuniversität Leoben | Tools: PyTorch, Scikit-learn, Python 3.8+

# Thank You!