

# 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

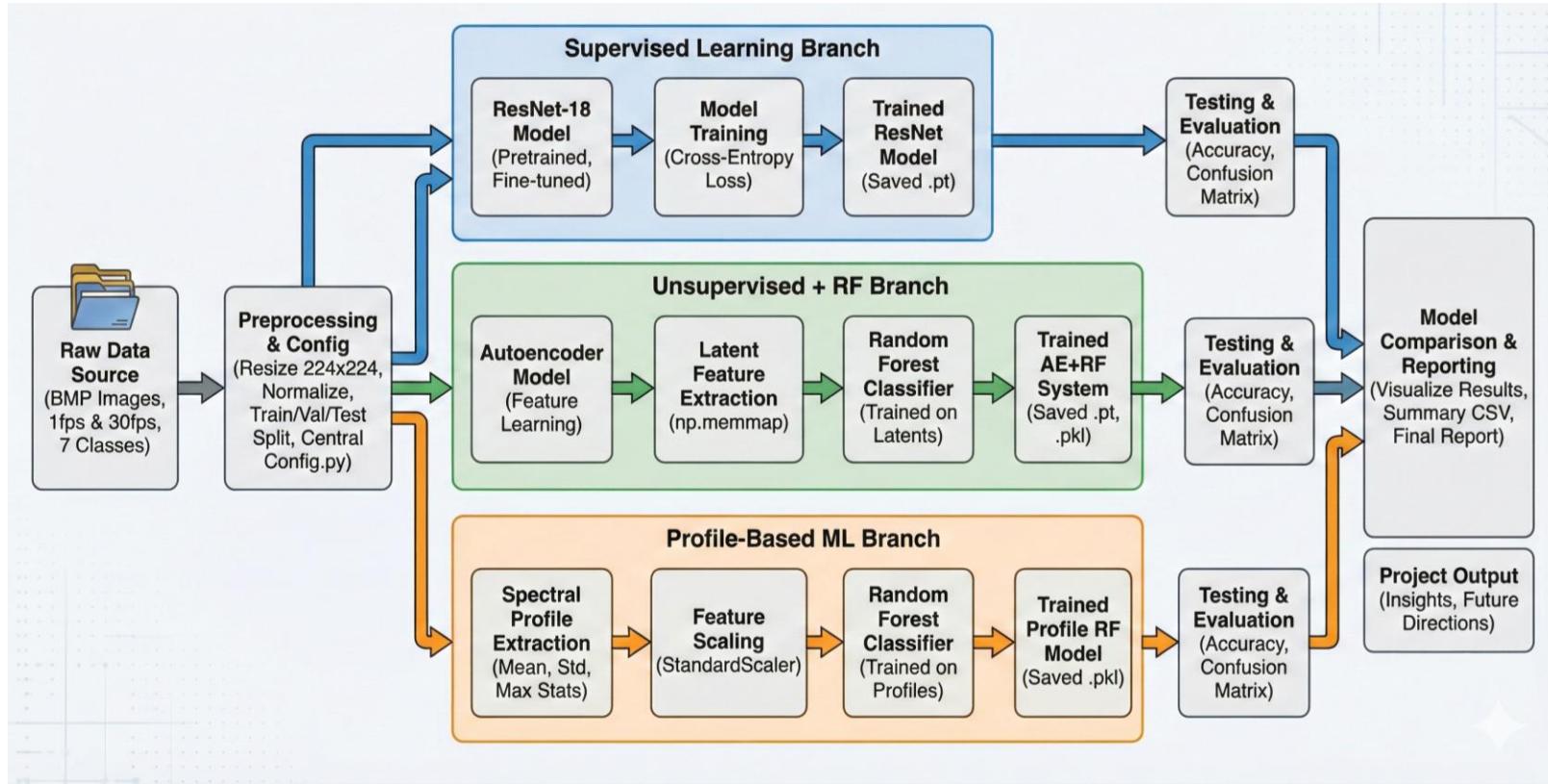
Autoencoder + Random Forest for feature learning

### 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

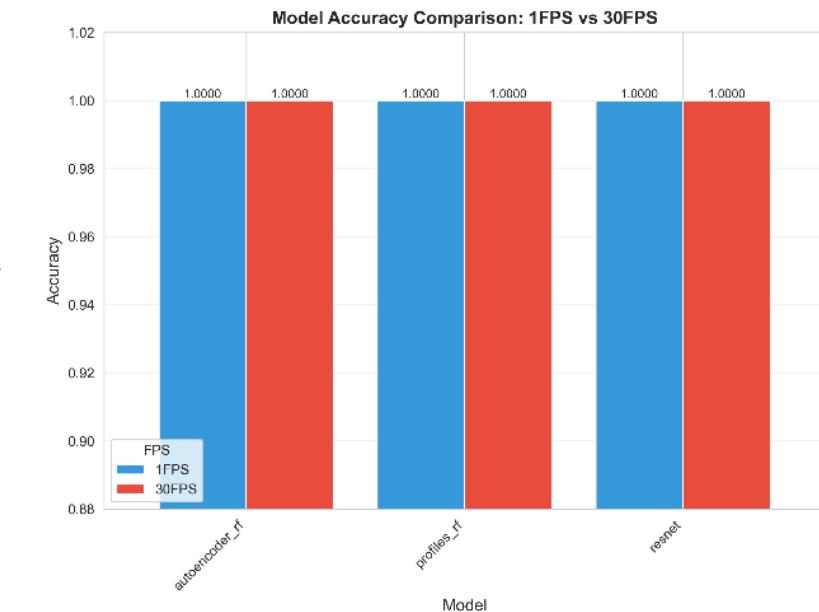
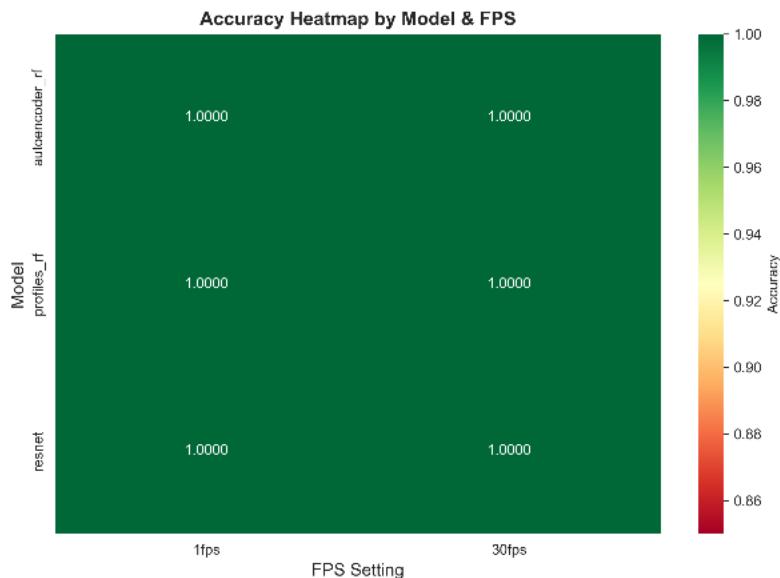
## Consistency

Identical results for both 1 FPS and 30 FPS datasets

## Inference Comparison

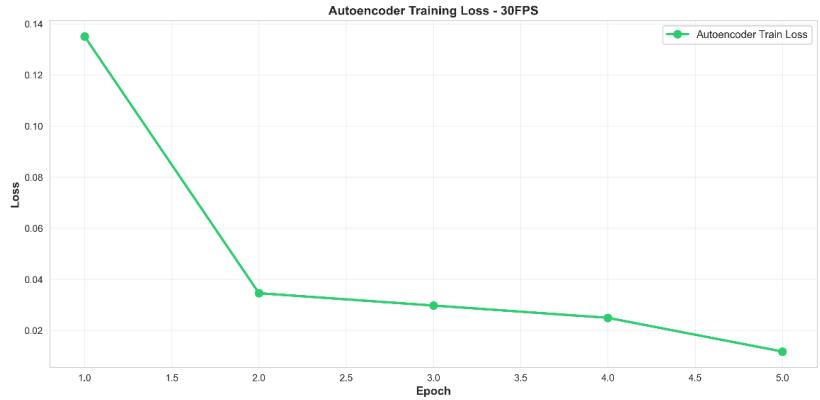
- **ResNet:** Fast, GPU-dependent training
- **Profiles RF:** Fastest, CPU-friendly

# Results Visualizations

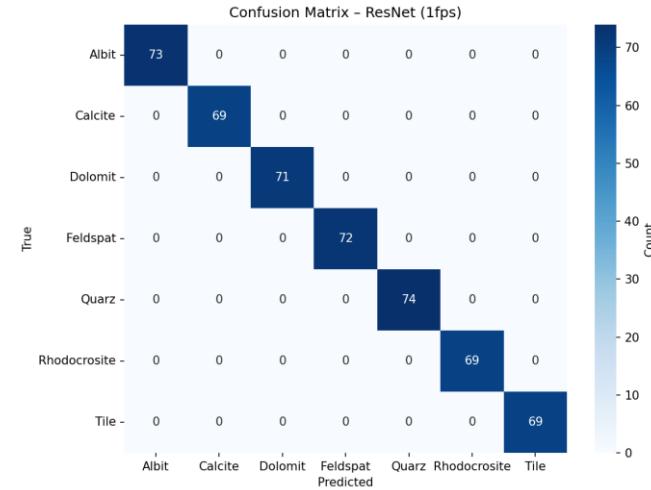


**Confusion Matrices:** Zero misclassifications across all 7 classes  
**Bar charts:** Charts showing 100% accuracy across all models

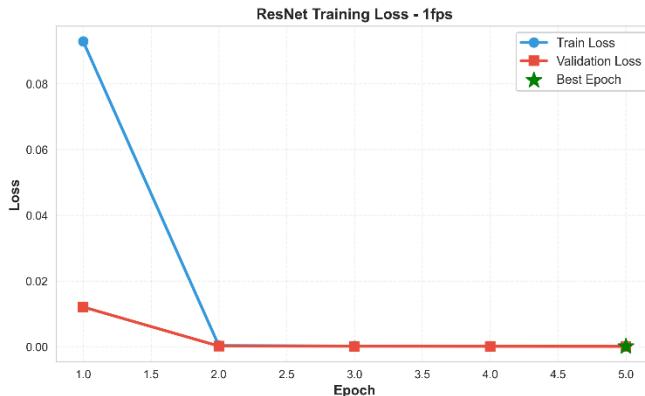
**(Cont.)**



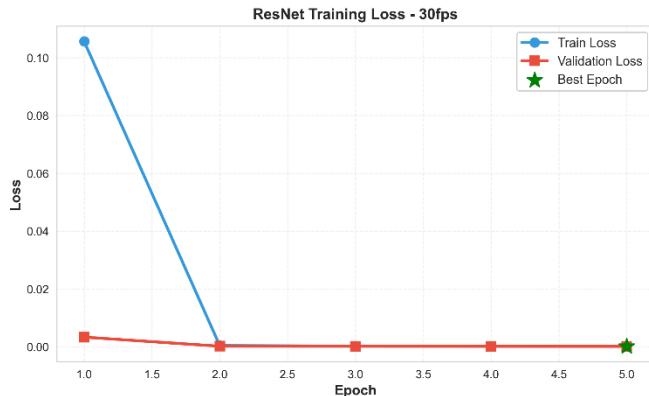
Autoencoder Training Loss Curve(30 FPS)



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 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 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 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!**